



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:05 AM GMT

PDB ID : 3KSC  
Title : Crystal structure of pea prolegumin, an 11S seed globulin from *Pisum sativum* L.  
Authors : Tandang-Silvas, M.R.G.; Fukuda, T.; Fukuda, C.; Prak, K.; Cabanos, C.; Kimura, A.; Itoh, T.; Mikami, B.; Maruyama, N.; Utsumi, S.  
Deposited on : 2009-11-21  
Resolution : 2.61 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865



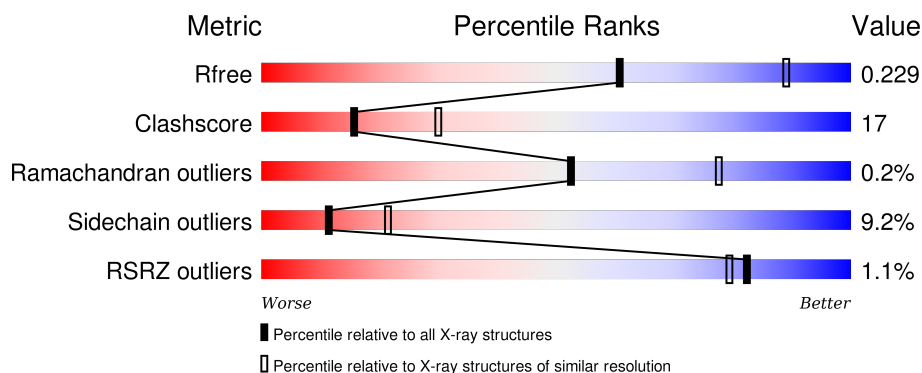
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	496	<div> <div>51%</div> <div>23%</div> <div>•</div> <div>23%</div> </div>
1	B	496	<div> <div>50%</div> <div>25%</div> <div>•</div> <div>23%</div> </div>
1	C	496	<div> <div>50%</div> <div>22%</div> <div>•</div> <div>24%</div> </div>
1	D	496	<div> <div>51%</div> <div>22%</div> <div>•</div> <div>24%</div> </div>
1	E	496	<div> <div>52%</div> <div>22%</div> <div>•</div> <div>23%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	496	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	503	-	-	X	-
3	GOL	B	504	-	-	X	X
3	GOL	B	505	-	-	X	-
3	GOL	B	506	-	-	X	X
3	GOL	C	499	-	-	X	X
3	GOL	C	500	-	-	-	X
3	GOL	D	499	-	-	X	-
3	GOL	F	499	-	-	X	-



## 2 Entry composition [i](#)

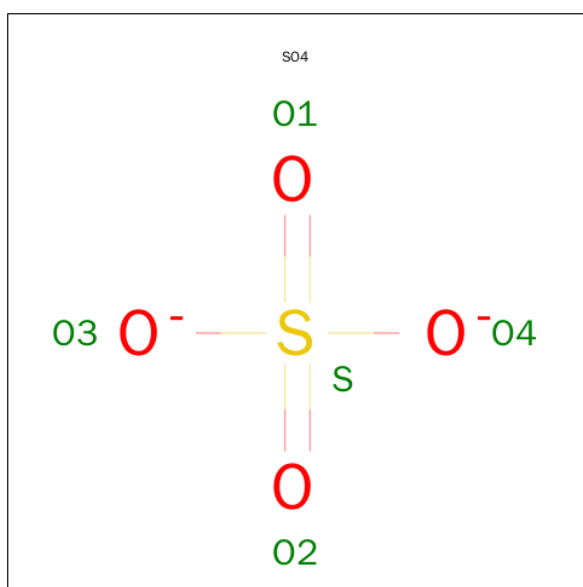
There are 4 unique types of molecules in this entry. The entry contains 18563 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called LegA class.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			3011	1886	556	560	9			
1	B	383	Total	C	N	O	S	0	0	0
			3039	1903	559	568	9			
1	C	375	Total	C	N	O	S	0	0	0
			2967	1859	545	554	9			
1	D	376	Total	C	N	O	S	0	0	0
			2980	1867	548	556	9			
1	E	383	Total	C	N	O	S	0	0	0
			3045	1910	563	563	9			
1	F	377	Total	C	N	O	S	0	2	0
			3007	1883	556	559	9			

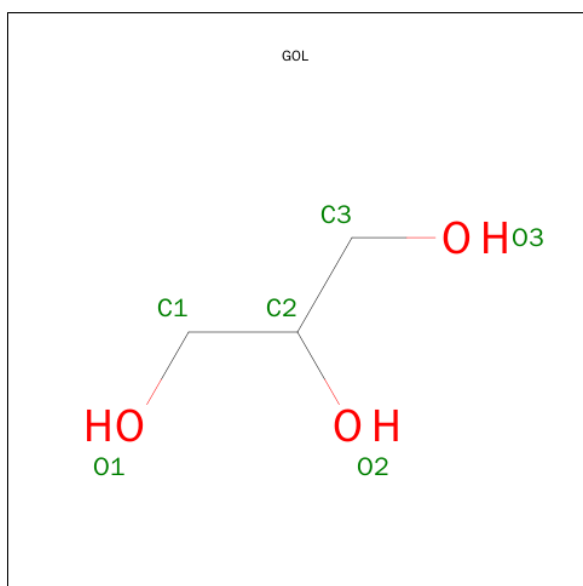
- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	53	Total O 53 53	0	0
4	B	73	Total O 73 73	0	0

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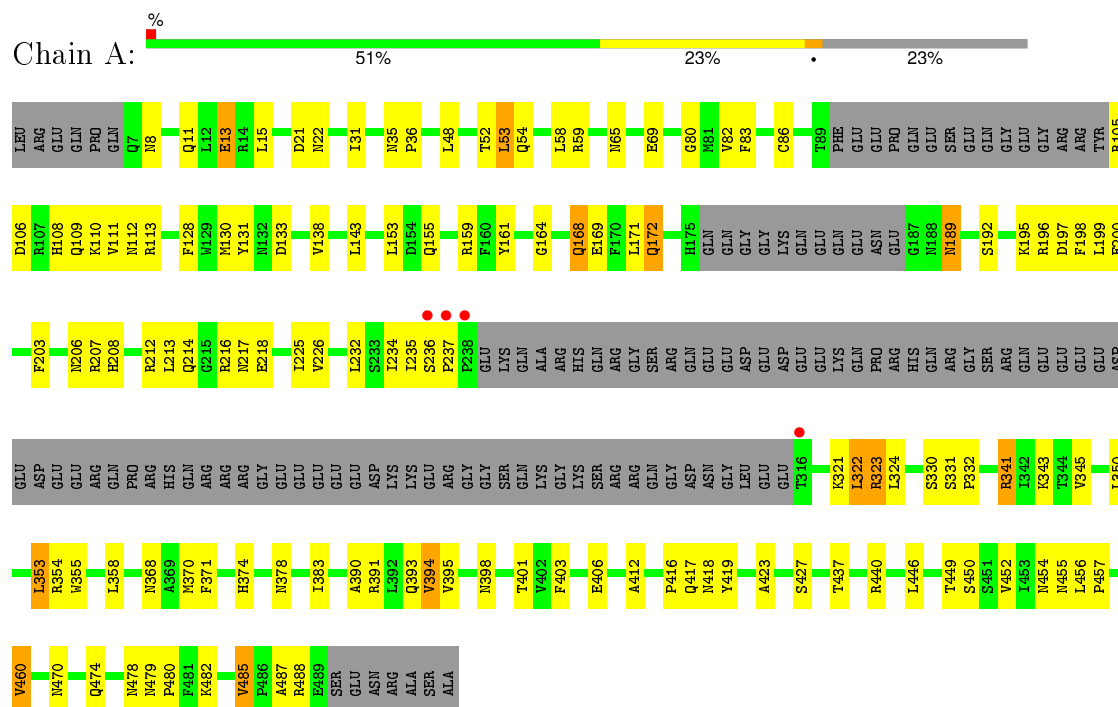
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	62	Total 62	O 62	0	0
4	D	60	Total 60	O 60	0	0
4	E	47	Total 47	O 47	0	0
4	F	46	Total 46	O 46	0	0



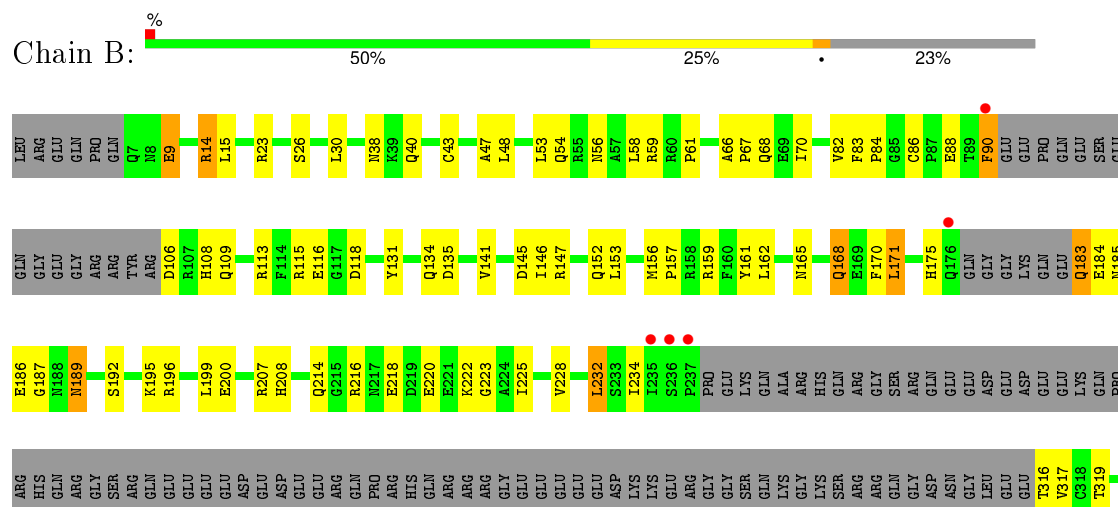
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

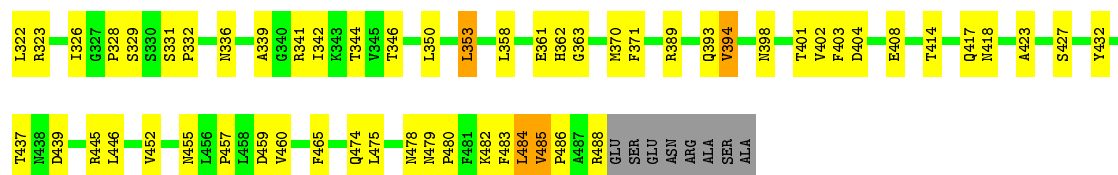
- Molecule 1: LegA class



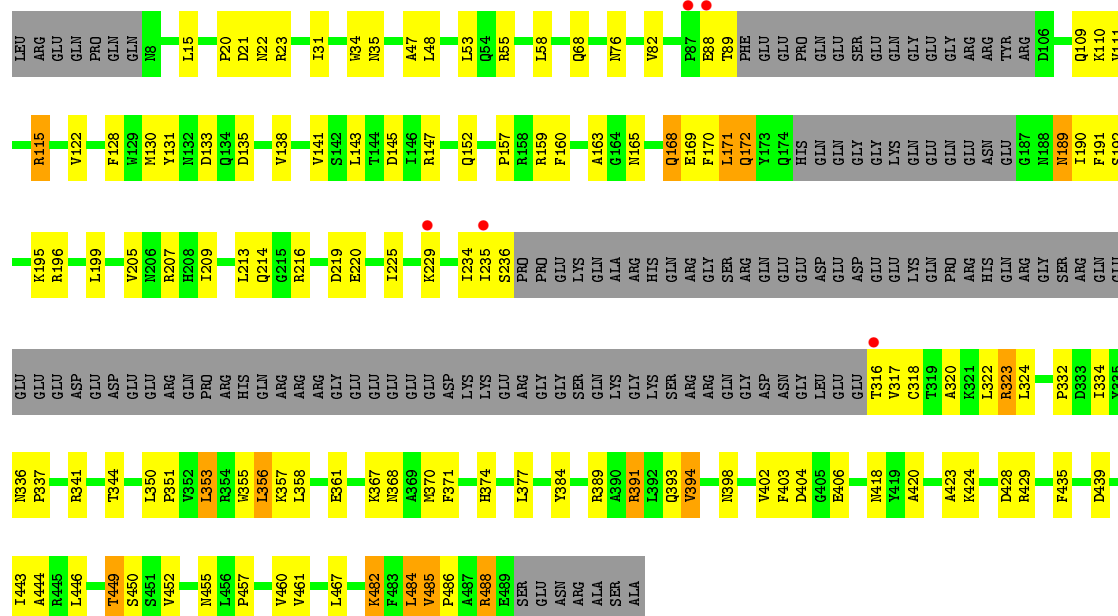
- Molecule 1: LegA class



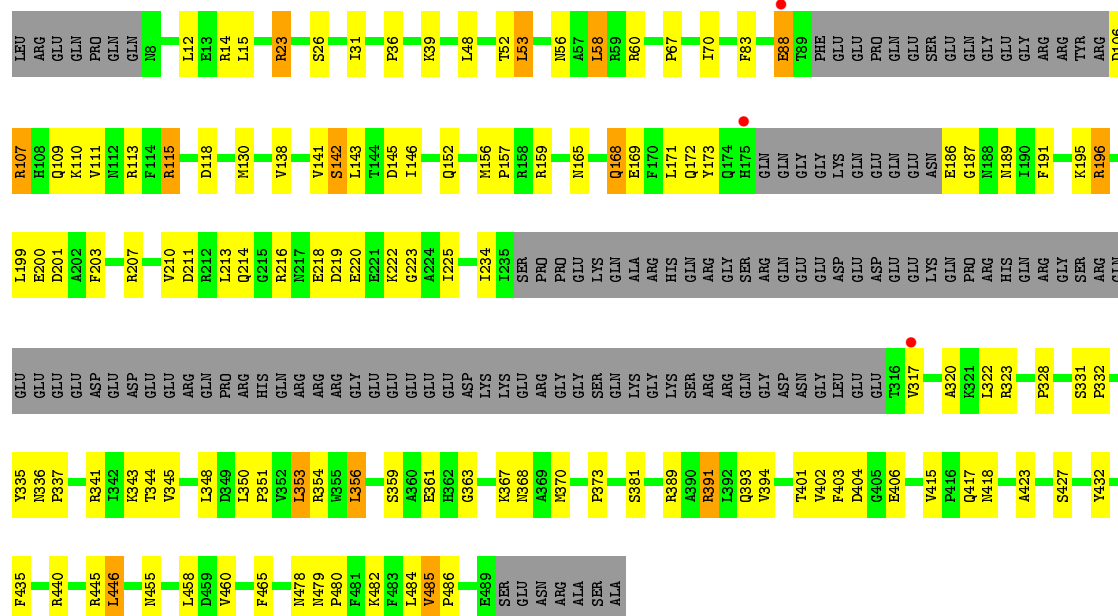




• Molecule 1: LegA class

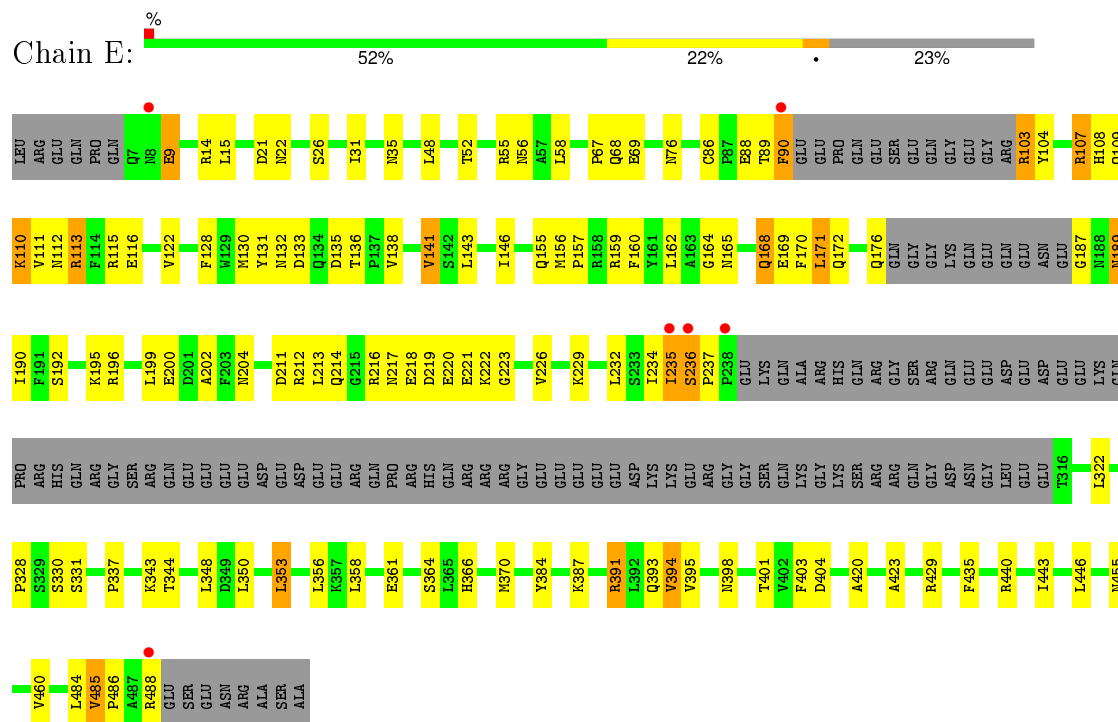


• Molecule 1: LegA class

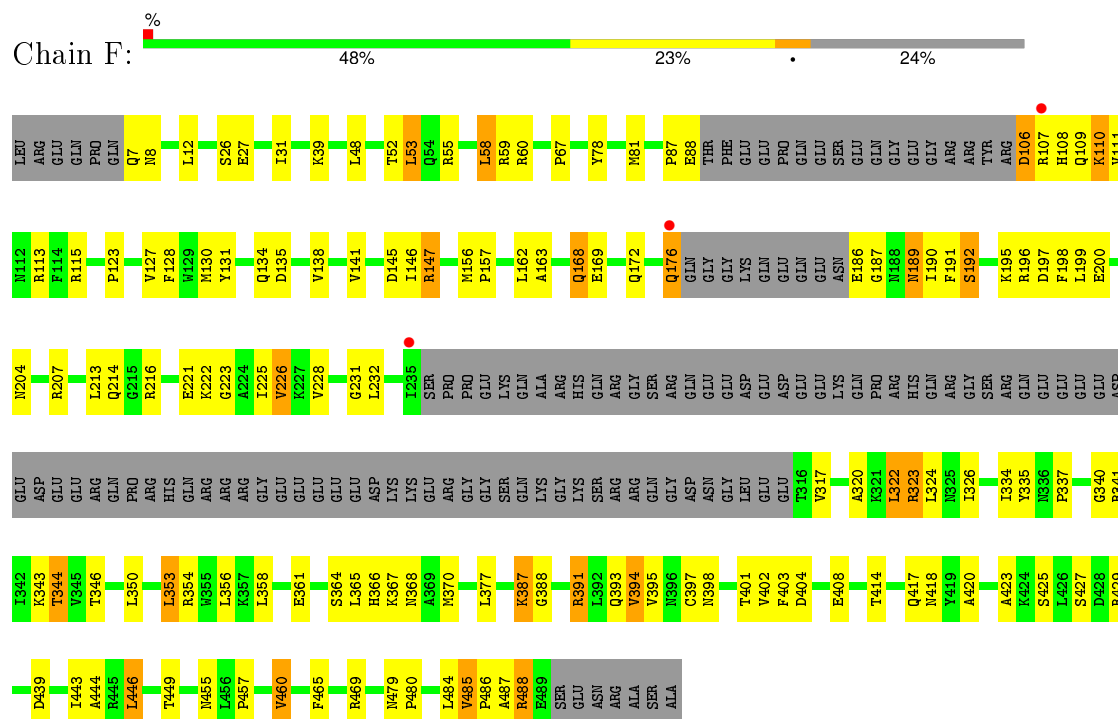




- Molecule 1: LegA class



- Molecule 1: LegA class





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.78Å 148.44Å 149.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.06 – 2.61 49.06 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.06-2.61) 99.3 (49.06-2.61)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.175 , 0.234 0.169 , 0.229	Depositor DCC
$R_{free}$ test set	4428 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 33.0	EDS
Estimated twinning fraction	0.069 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	2 of 88227 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18563	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.32	0/3070	0.51	0/4155
1	B	0.33	0/3098	0.51	0/4192
1	C	0.33	0/3023	0.52	0/4090
1	D	0.32	0/3037	0.51	0/4109
1	E	0.33	0/3106	0.51	0/4203
1	F	0.31	0/3068	0.51	0/4148
All	All	0.32	0/18402	0.51	0/24897

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3011	0	2962	108	0
1	B	3039	0	2979	120	0
1	C	2967	0	2920	114	0
1	D	2980	0	2928	118	0
1	E	3045	0	2995	109	0
1	F	3007	0	2958	112	0
2	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	30	0	0	0	0
2	C	10	0	0	0	0
2	D	5	0	0	1	0
2	E	10	0	0	0	0
3	A	12	0	16	2	0
3	B	30	0	40	27	0
3	C	24	0	32	11	0
3	D	18	0	24	8	0
3	E	6	0	8	0	0
3	F	18	0	24	7	0
4	A	53	0	0	9	0
4	B	73	0	0	5	0
4	C	62	0	0	1	0
4	D	60	0	0	1	0
4	E	47	0	0	1	0
4	F	46	0	0	3	0
All	All	18563	0	17886	616	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (616) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:ILE:HG21	1:E:169:GLU:HG2	1.27	1.16
1:F:186:GLU:HG3	1:F:187:GLY:H	1.17	1.08
1:D:391:ARG:HG3	1:D:391:ARG:HH11	1.15	1.04
1:D:328:PRO:HG3	3:D:500:GOL:H31	1.41	1.03
1:F:31:ILE:HG21	1:F:169:GLU:HG2	1.41	1.00
1:D:31:ILE:HG21	1:D:169:GLU:HG2	1.45	0.96
1:C:344:THR:HG22	1:C:361:GLU:HG3	1.48	0.95
1:B:393:GLN:HE22	1:C:195:LYS:H	1.03	0.95
1:D:455:ASN:HD22	1:F:109:GLN:HG3	1.31	0.95
3:B:503:GOL:H2	1:E:115:ARG:HG2	1.48	0.94
1:C:229:LYS:HD2	1:C:229:LYS:H	1.30	0.94
1:B:455:ASN:HD22	1:C:109:GLN:HG3	1.34	0.92
1:E:103:ARG:HH22	1:F:469:ARG:HD2	1.33	0.91
1:A:13:GLU:H	1:A:13:GLU:CD	1.76	0.89
1:C:31:ILE:HG21	1:C:169:GLU:HG2	1.54	0.89
1:A:86:CYS:HB2	1:A:109:GLN:NE2	1.89	0.88
1:D:391:ARG:CG	1:D:391:ARG:HH11	1.86	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:323:ARG:HH12	3:F:498:GOL:H31	1.40	0.86
1:F:195[B]:LYS:HE2	3:F:499:GOL:H31	1.57	0.84
1:E:370:MET:HB2	1:E:423:ALA:O	1.77	0.84
1:D:70:ILE:HG12	1:D:142:SER:HB3	1.57	0.84
1:B:113:ARG:HD3	3:B:503:GOL:H32	1.61	0.83
1:E:350:LEU:HB3	1:E:353:LEU:HD22	1.61	0.82
1:D:393:GLN:HE22	1:F:195[A]:LYS:H	1.26	0.82
1:E:214:GLN:NE2	1:E:216:ARG:HE	1.78	0.82
1:D:393:GLN:HE22	1:F:195[B]:LYS:H	1.27	0.81
1:E:103:ARG:HH12	1:F:469:ARG:HH11	1.26	0.81
1:A:31:ILE:HG21	1:A:169:GLU:HG2	1.62	0.81
1:B:146:ILE:HD11	1:B:157:PRO:HG3	1.63	0.81
1:D:88:GLU:HG2	1:E:455:ASN:HD21	1.44	0.80
1:E:214:GLN:HE21	1:E:216:ARG:HE	1.29	0.80
1:A:236:SER:HB2	1:A:237:PRO:HA	1.62	0.79
1:F:186:GLU:HG3	1:F:187:GLY:N	1.98	0.79
3:B:504:GOL:H32	1:E:55:ARG:NE	1.98	0.79
1:B:362:HIS:HE1	3:B:504:GOL:H2	1.48	0.78
3:B:504:GOL:H32	1:E:55:ARG:HE	1.48	0.78
1:C:21:ASP:OD2	1:C:35:ASN:HB2	1.83	0.78
1:A:393:GLN:HE22	1:B:195:LYS:H	1.30	0.77
1:B:389:ARG:HD3	3:B:505:GOL:H11	1.64	0.77
1:B:362:HIS:CE1	3:B:504:GOL:H2	2.20	0.77
1:D:31:ILE:CG2	1:D:169:GLU:HG2	2.15	0.76
1:B:328:PRO:HG3	3:B:504:GOL:H11	1.66	0.76
1:B:228:VAL:HG11	1:B:232:LEU:HD23	1.68	0.75
1:D:196:ARG:HE	1:D:207:ARG:HE	1.32	0.75
1:D:67:PRO:HG2	1:D:145:ASP:HB3	1.67	0.75
1:F:370:MET:HB2	1:F:423:ALA:O	1.86	0.75
1:B:165:ASN:OD1	1:B:187:GLY:HA2	1.86	0.75
1:A:332:PRO:HG3	1:A:341:ARG:NH2	2.02	0.74
1:D:130:MET:HE1	1:D:138:VAL:HG11	1.69	0.74
1:D:88:GLU:HG2	1:E:455:ASN:ND2	2.02	0.73
1:D:389:ARG:HH21	3:D:499:GOL:H12	1.51	0.73
1:A:212:ARG:HH12	1:A:217:ASN:HD22	1.37	0.73
1:E:344:THR:HG22	1:E:361:GLU:HG3	1.69	0.73
1:F:214:GLN:NE2	1:F:216:ARG:HE	1.86	0.72
1:C:370:MET:HB2	1:C:423:ALA:O	1.90	0.71
1:E:236:SER:H	1:E:237:PRO:CD	2.03	0.71
1:A:394:VAL:HG13	1:A:403:PHE:HB3	1.72	0.71
1:B:214:GLN:NE2	1:B:216:ARG:HE	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:ARG:HG3	1:D:391:ARG:NH1	1.96	0.70
1:C:214:GLN:NE2	1:C:216:ARG:HE	1.89	0.70
1:B:370:MET:HB2	1:B:423:ALA:O	1.92	0.70
1:C:68:GLN:HE21	1:C:159:ARG:HH21	1.37	0.69
3:B:503:GOL:C2	1:E:115:ARG:HG2	2.21	0.69
1:B:196:ARG:HD2	1:B:207:ARG:NE	2.06	0.69
1:C:323:ARG:HH22	3:C:501:GOL:H2	1.55	0.69
1:D:196:ARG:HG3	1:D:210:VAL:HG11	1.75	0.69
1:E:236:SER:H	1:E:237:PRO:HD2	1.58	0.69
1:D:344:THR:HG22	1:D:361:GLU:HG3	1.75	0.69
1:A:53:LEU:HD22	1:A:225:ILE:HD13	1.73	0.69
1:C:394:VAL:HG13	1:C:403:PHE:HB3	1.75	0.69
1:F:394:VAL:HG13	1:F:403:PHE:HB3	1.75	0.68
1:C:449:THR:HB	1:C:482:LYS:HA	1.76	0.68
1:E:76:ASN:HD22	1:E:115:ARG:HA	1.57	0.68
1:C:374:HIS:NE2	3:C:500:GOL:H2	2.09	0.68
1:A:398:ASN:ND2	1:B:171:LEU:HG	2.09	0.68
1:B:394:VAL:HG13	1:B:403:PHE:HB3	1.76	0.68
1:B:393:GLN:HE22	1:C:195:LYS:N	1.85	0.68
1:B:457:PRO:HB2	1:B:460:VAL:HG13	1.74	0.67
1:C:229:LYS:HD2	1:C:229:LYS:N	2.08	0.67
1:B:196:ARG:NH1	1:B:207:ARG:HE	1.90	0.67
1:A:86:CYS:HB2	1:A:109:GLN:HE22	1.58	0.67
1:B:353:LEU:HG	1:B:358:LEU:O	1.94	0.67
1:D:109:GLN:HG3	1:E:455:ASN:HD22	1.59	0.67
1:F:189:ASN:ND2	1:F:192:SER:H	1.91	0.67
1:C:229:LYS:CD	1:C:229:LYS:H	2.07	0.67
1:F:67:PRO:HG2	1:F:145:ASP:HB3	1.76	0.66
1:B:196:ARG:HH11	1:B:207:ARG:HE	1.43	0.66
1:A:105:ARG:N	1:A:106:ASP:HA	2.10	0.66
1:E:110:LYS:HE3	1:E:112:ASN:HD21	1.61	0.66
3:B:507:GOL:H2	1:E:429:ARG:NH1	2.11	0.66
1:F:172:GLN:HG2	4:F:508:HOH:O	1.95	0.66
1:F:195[A]:LYS:HE2	3:F:499:GOL:O3	1.96	0.66
1:D:391:ARG:HH21	3:F:499:GOL:H32	1.59	0.65
1:F:162:LEU:HA	1:F:190:ILE:HD11	1.78	0.65
1:B:401:THR:HG21	1:B:404:ASP:HB2	1.77	0.65
1:B:187:GLY:HA3	4:B:548:HOH:O	1.97	0.65
1:D:195:LYS:HD2	1:E:391:ARG:HH21	1.60	0.65
3:B:507:GOL:O3	1:E:387:LYS:HE2	1.96	0.65
1:A:460:VAL:HG12	1:B:232:LEU:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:548:HOH:O	1:B:208:HIS:HE1	1.79	0.65
1:C:207:ARG:HE	3:C:502:GOL:H32	1.61	0.64
1:B:168:GLN:OE1	1:B:170:PHE:HB2	1.97	0.64
1:C:370:MET:HG3	1:C:485:VAL:HG13	1.78	0.63
3:B:503:GOL:H2	1:E:115:ARG:CG	2.26	0.63
1:B:108:HIS:HD2	1:B:109:GLN:O	1.82	0.63
1:E:103:ARG:HH12	1:F:469:ARG:NH1	1.96	0.63
1:B:401:THR:CG2	1:B:404:ASP:HB2	2.29	0.63
1:E:165:ASN:OD1	1:E:187:GLY:HA2	1.99	0.63
1:C:391:ARG:NH1	1:C:404:ASP:OD1	2.32	0.63
1:E:214:GLN:HE22	1:E:216:ARG:HH11	1.46	0.63
1:A:212:ARG:NH1	1:A:217:ASN:HD22	1.95	0.63
1:F:350:LEU:HB3	1:F:353:LEU:HD22	1.79	0.63
1:F:353:LEU:HG	1:F:358:LEU:O	1.99	0.63
1:D:15:LEU:HB2	1:D:403:PHE:HB2	1.81	0.63
1:C:323:ARG:HH11	1:C:323:ARG:HB3	1.64	0.62
1:A:15:LEU:HB2	1:A:403:PHE:HB2	1.82	0.62
1:E:22:ASN:CG	1:E:172:GLN:HE22	2.03	0.62
1:A:321:LYS:HE2	1:A:323:ARG:O	2.00	0.62
1:B:118:ASP:OD2	1:B:323:ARG:HD2	2.00	0.61
1:E:143:LEU:HD13	1:E:435:PHE:CB	2.31	0.61
1:B:59:ARG:HH21	3:B:506:GOL:H31	1.64	0.61
1:D:348:LEU:HD21	1:D:440:ARG:NH1	2.15	0.61
1:B:115:ARG:HG2	4:B:529:HOH:O	2.01	0.61
1:A:457:PRO:HB2	1:A:460:VAL:HG13	1.83	0.61
1:C:207:ARG:NE	3:C:502:GOL:H32	2.15	0.61
1:D:317:VAL:HG22	1:D:320:ALA:HB2	1.83	0.60
1:E:162:LEU:HD22	1:E:190:ILE:HD11	1.83	0.60
1:A:393:GLN:OE1	1:B:195:LYS:HG2	2.00	0.60
1:D:370:MET:HG3	1:D:485:VAL:HG13	1.83	0.60
1:F:370:MET:HG3	1:F:485:VAL:HG13	1.84	0.60
1:C:234:ILE:HG22	1:C:236:SER:H	1.65	0.60
1:D:363:GLY:HA3	1:D:432:TYR:CZ	2.36	0.60
1:D:26:SER:HB3	1:D:223:GLY:HA3	1.84	0.60
1:A:195:LYS:HG3	4:A:509:HOH:O	2.01	0.60
1:B:445:ARG:NH2	1:B:482:LYS:HE2	2.17	0.60
1:D:331:SER:O	1:D:343:LYS:HE2	2.02	0.60
1:C:15:LEU:HB2	1:C:403:PHE:HB2	1.84	0.60
1:A:108:HIS:HD2	1:A:109:GLN:O	1.85	0.60
1:F:370:MET:CB	1:F:423:ALA:O	2.50	0.60
1:D:214:GLN:HE21	1:D:216:ARG:HE	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:ARG:NH1	1:C:323:ARG:HB3	2.17	0.59
1:B:161:TYR:HE1	4:B:562:HOH:O	1.84	0.59
1:C:168:GLN:OE1	1:C:170:PHE:HB2	2.00	0.59
1:C:393:GLN:HG2	1:C:404:ASP:OD1	2.02	0.59
1:F:88:GLU:HB3	1:F:108:HIS:O	2.01	0.59
1:E:443:ILE:O	1:E:443:ILE:HG13	1.99	0.59
1:A:131:TYR:CE2	1:A:133:ASP:HB3	2.39	0.58
1:E:31:ILE:CG2	1:E:169:GLU:HG2	2.18	0.58
1:A:440:ARG:NH2	1:B:316:THR:HG23	2.19	0.58
1:D:200:GLU:OE2	1:D:207:ARG:HD3	2.04	0.57
1:E:212:ARG:NH1	1:E:217:ASN:HD22	2.03	0.57
1:C:449:THR:HG22	1:C:450:SER:N	2.19	0.57
1:D:196:ARG:HG3	1:D:210:VAL:CG1	2.34	0.57
1:B:362:HIS:CE1	3:B:504:GOL:H12	2.40	0.57
1:A:455:ASN:HB3	1:B:109:GLN:HG3	1.86	0.57
1:C:76:ASN:ND2	1:C:115:ARG:HB3	2.19	0.57
1:E:353:LEU:HG	1:E:358:LEU:O	2.05	0.57
1:A:371:PHE:CE1	1:A:374:HIS:HE1	2.21	0.57
1:D:58:LEU:HD13	1:D:60:ARG:HG2	1.87	0.57
1:A:350:LEU:HB3	1:A:353:LEU:HD22	1.86	0.57
1:B:344:THR:HG22	1:B:361:GLU:HG3	1.87	0.57
1:A:189:ASN:ND2	1:A:192:SER:H	2.03	0.57
1:C:361:GLU:OE2	3:C:500:GOL:O1	2.22	0.56
1:A:196:ARG:HD2	1:A:207:ARG:HD2	1.87	0.56
1:C:189:ASN:ND2	1:C:192:SER:H	2.03	0.56
1:A:189:ASN:HD22	1:A:189:ASN:C	2.09	0.56
1:A:427:SER:HB3	3:A:500:GOL:H2	1.86	0.56
1:B:218:GLU:HG3	1:B:222:LYS:HD2	1.88	0.56
1:B:70:ILE:HD13	3:B:506:GOL:H12	1.88	0.56
1:E:195:LYS:H	1:F:393:GLN:HE22	1.52	0.56
1:E:370:MET:CB	1:E:423:ALA:O	2.53	0.56
1:F:59:ARG:HD2	4:F:524:HOH:O	2.06	0.56
1:D:159:ARG:HB2	1:D:168:GLN:HG3	1.89	0.55
1:E:214:GLN:HE21	1:E:216:ARG:NE	2.02	0.55
1:E:143:LEU:HD13	1:E:435:PHE:HB2	1.89	0.55
1:B:200:GLU:OE2	1:B:207:ARG:HD3	2.06	0.55
1:F:58:LEU:HB3	1:F:226:VAL:HG12	1.89	0.55
1:B:329:SER:HB2	4:E:540:HOH:O	2.06	0.55
1:D:107:ARG:H	1:D:107:ARG:NH2	2.04	0.55
1:B:455:ASN:ND2	1:C:109:GLN:HG3	2.13	0.55
1:B:389:ARG:HG2	1:B:408:GLU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:MET:CB	1:C:423:ALA:O	2.55	0.55
1:F:340:GLY:HA3	1:F:364:SER:O	2.05	0.55
1:E:214:GLN:NE2	1:E:216:ARG:NE	2.54	0.55
1:A:200:GLU:OE2	1:A:207:ARG:HD3	2.06	0.55
1:F:53:LEU:HD22	1:F:225:ILE:HD13	1.88	0.55
1:A:427:SER:CB	3:A:500:GOL:H2	2.36	0.55
1:B:336:ASN:HB3	1:B:339:ALA:HB3	1.87	0.55
1:B:40:GLN:HE21	1:B:414:THR:H	1.53	0.55
1:F:26:SER:HB2	1:F:223:GLY:HA3	1.89	0.55
1:F:346:THR:HB	1:F:439:ASP:O	2.06	0.55
1:E:131:TYR:CG	1:E:232:LEU:HD12	2.43	0.54
1:D:478:ASN:HB3	1:F:204:ASN:HB3	1.90	0.54
1:D:391:ARG:CG	1:D:391:ARG:NH1	2.56	0.54
1:B:113:ARG:CD	3:B:503:GOL:H32	2.36	0.54
1:A:370:MET:HB2	1:A:423:ALA:O	2.06	0.54
1:B:183:GLN:OE1	1:B:185:ASN:HB3	2.07	0.54
1:A:370:MET:HG3	1:A:485:VAL:HG13	1.89	0.54
1:E:15:LEU:HB2	1:E:403:PHE:HB2	1.88	0.54
1:F:427:SER:OG	3:F:497:GOL:H2	2.07	0.54
1:A:111:VAL:HG11	1:A:234:ILE:HG22	1.90	0.54
1:A:169:GLU:HG3	4:A:542:HOH:O	2.07	0.54
1:D:348:LEU:HD11	1:D:440:ARG:NH2	2.23	0.54
1:E:196:ARG:HD3	1:E:211:ASP:OD1	2.08	0.54
1:D:196:ARG:NH2	1:D:216:ARG:NH1	2.56	0.54
1:D:332:PRO:HG3	1:D:341:ARG:CZ	2.38	0.53
1:B:134:GLN:NE2	1:E:115:ARG:HE	2.07	0.53
1:D:196:ARG:NE	1:D:207:ARG:HE	2.03	0.53
1:D:417:GLN:O	1:D:418:ASN:HB2	2.08	0.53
1:D:370:MET:CB	1:D:423:ALA:O	2.56	0.53
1:C:131:TYR:CE2	1:C:133:ASP:HB3	2.43	0.53
1:A:22:ASN:CG	1:A:172:GLN:HE22	2.11	0.53
1:B:26:SER:HB3	1:B:223:GLY:HA3	1.90	0.53
1:C:68:GLN:NE2	1:C:159:ARG:HH21	2.05	0.53
1:F:370:MET:CG	1:F:485:VAL:HG13	2.39	0.53
1:E:159:ARG:HB2	1:E:168:GLN:HG3	1.90	0.53
1:B:362:HIS:CE1	3:B:504:GOL:C2	2.91	0.53
1:B:9:GLU:O	1:B:43:CYS:HB2	2.09	0.53
1:D:458:LEU:HB2	1:F:106:ASP:HB3	1.90	0.53
1:A:13:GLU:CD	1:A:13:GLU:N	2.53	0.52
1:F:222:LYS:HE3	1:F:226:VAL:CG2	2.39	0.52
1:E:88:GLU:OE1	1:E:107:ARG:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:PRO:HB2	3:C:499:GOL:H11	1.90	0.52
1:E:164:GLY:HA2	1:E:218:GLU:OE1	2.09	0.52
1:E:168:GLN:HG2	1:E:170:PHE:H	1.74	0.52
1:E:109:GLN:HG3	1:F:455:ASN:HD22	1.74	0.52
1:E:213:LEU:HD12	1:F:465:PHE:CD1	2.44	0.52
1:B:189:ASN:C	1:B:189:ASN:HD22	2.13	0.52
1:C:53:LEU:HD22	1:C:225:ILE:HG21	1.91	0.52
1:B:427:SER:HB3	3:B:505:GOL:H32	1.92	0.52
1:E:219:ASP:OD1	1:E:221:GLU:HB2	2.10	0.52
1:F:457:PRO:HB2	1:F:460:VAL:HG13	1.92	0.52
1:F:55[B]:ARG:HG3	1:F:134:GLN:O	2.10	0.52
1:C:131:TYR:HE2	1:C:133:ASP:HB3	1.73	0.52
1:B:189:ASN:ND2	1:B:192:SER:H	2.08	0.52
1:D:200:GLU:HG3	1:D:210:VAL:HG21	1.91	0.52
1:D:111:VAL:HG21	1:D:234:ILE:HG21	1.92	0.51
1:D:214:GLN:NE2	1:D:216:ARG:HE	2.08	0.51
1:B:350:LEU:HB3	1:B:353:LEU:HD22	1.92	0.51
1:A:437:THR:OG1	1:B:152:GLN:NE2	2.43	0.51
1:C:207:ARG:HE	3:C:502:GOL:C3	2.23	0.51
1:A:159:ARG:HB2	1:A:168:GLN:HG3	1.92	0.51
1:E:26:SER:HB3	1:E:223:GLY:HA3	1.92	0.51
1:F:195[B]:LYS:HE2	3:F:499:GOL:C3	2.35	0.51
1:F:88:GLU:OE2	1:F:107:ARG:HB3	2.10	0.51
1:A:206:ASN:OD1	1:A:208:HIS:HB3	2.11	0.51
1:B:474:GLN:HE21	1:B:478:ASN:HD21	1.58	0.51
1:A:189:ASN:HD22	1:A:192:SER:H	1.58	0.51
1:A:341:ARG:HD2	4:A:512:HOH:O	2.10	0.51
1:C:190:ILE:HD12	1:C:191:PHE:N	2.26	0.51
1:D:118:ASP:OD2	1:D:323:ARG:HD2	2.11	0.51
1:A:330:SER:HB2	1:A:343:LYS:HE2	1.92	0.51
1:F:195[B]:LYS:O	1:F:198:PHE:HB2	2.11	0.51
1:D:370:MET:HG3	1:D:485:VAL:CG1	2.40	0.51
1:E:103:ARG:NH2	1:F:469:ARG:HD2	2.15	0.51
1:A:164:GLY:HA2	1:A:218:GLU:OE1	2.10	0.51
1:F:131:TYR:CG	1:F:232:LEU:HD12	2.46	0.51
1:B:131:TYR:CZ	1:B:232:LEU:HB2	2.47	0.50
1:E:236:SER:N	1:E:237:PRO:CD	2.73	0.50
1:C:334:ILE:CD1	1:C:482:LYS:HG2	2.42	0.50
1:E:68:GLN:HB2	1:E:122:VAL:HB	1.94	0.50
1:A:54:GLN:HG3	4:A:537:HOH:O	2.10	0.50
1:A:378:ASN:HA	1:A:417:GLN:NE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ASN:ND2	1:B:109:GLN:HG3	2.26	0.50
1:D:106:ASP:HA	1:D:107:ARG:NH2	2.26	0.50
1:D:12:LEU:HD23	1:D:39:LYS:HD2	1.94	0.50
1:C:159:ARG:O	1:C:168:GLN:HG3	2.11	0.50
1:F:189:ASN:C	1:F:189:ASN:HD22	2.14	0.50
1:D:83:PHE:HD2	1:D:110:LYS:HZ3	1.58	0.50
1:C:147:ARG:HH11	1:C:147:ARG:HG3	1.77	0.50
1:F:228:VAL:HG12	1:F:231:GLY:H	1.77	0.50
1:D:23:ARG:HH11	1:D:23:ARG:HG2	1.76	0.50
1:C:22:ASN:CG	1:C:172:GLN:HE22	2.15	0.50
1:A:390:ALA:O	1:A:406:GLU:HA	2.11	0.50
1:B:67:PRO:HG2	1:B:145:ASP:HB3	1.93	0.50
1:A:214:GLN:HE22	1:A:216:ARG:HH11	1.60	0.49
1:A:113:ARG:HH21	1:A:113:ARG:HB3	1.76	0.49
1:A:59:ARG:HB3	1:A:130:MET:HB2	1.95	0.49
1:C:334:ILE:HD11	1:C:482:LYS:HG2	1.94	0.49
1:B:38:ASN:ND2	4:B:546:HOH:O	2.45	0.49
1:C:31:ILE:HG21	1:C:169:GLU:CG	2.33	0.49
1:B:362:HIS:HE1	3:B:504:GOL:C2	2.23	0.49
1:F:394:VAL:HA	1:F:420:ALA:O	2.11	0.49
1:E:90:PHE:CD1	1:E:90:PHE:C	2.85	0.49
1:D:393:GLN:NE2	1:F:195[A]:LYS:H	2.01	0.49
1:E:235:ILE:HD13	1:E:235:ILE:H	1.78	0.49
1:F:350:LEU:O	1:F:353:LEU:HB2	2.12	0.49
1:F:195[A]:LYS:HD3	1:F:197:ASP:HB2	1.94	0.49
1:C:394:VAL:HG22	1:C:402:VAL:CG2	2.42	0.49
1:D:109:GLN:HG3	1:E:455:ASN:ND2	2.26	0.49
1:B:452:VAL:HA	1:C:82:VAL:HG11	1.94	0.49
1:F:190:ILE:HD12	1:F:191:PHE:H	1.78	0.49
1:F:487:ALA:HA	1:F:488:ARG:NH1	2.28	0.49
1:A:83:PHE:HE2	1:A:322:LEU:HD21	1.78	0.48
1:F:189:ASN:ND2	1:F:192:SER:N	2.61	0.48
1:D:393:GLN:NE2	1:F:195[B]:LYS:H	2.03	0.48
1:E:165:ASN:O	1:E:220:GLU:HG2	2.13	0.48
1:F:326:ILE:HA	1:F:343:LYS:HD2	1.95	0.48
1:E:113:ARG:HG3	1:E:237:PRO:HG2	1.95	0.48
1:A:195:LYS:HD2	1:C:391:ARG:NH2	2.29	0.48
1:B:393:GLN:OE1	1:C:195:LYS:HG3	2.14	0.48
1:B:394:VAL:HG22	1:B:402:VAL:CG2	2.44	0.48
1:D:458:LEU:HB2	1:F:106:ASP:CB	2.44	0.48
1:F:387:LYS:HG3	1:F:388:GLY:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:PRO:HA	1:F:356:LEU:HD22	1.95	0.48
1:F:128:PHE:CZ	1:F:130:MET:HG3	2.48	0.48
1:D:195:LYS:HD2	1:E:391:ARG:NH2	2.27	0.48
1:D:363:GLY:HA3	1:D:432:TYR:CE1	2.49	0.48
1:B:232:LEU:HD12	1:B:234:ILE:HD13	1.96	0.48
1:D:335:TYR:HD1	1:D:341:ARG:HB3	1.79	0.48
1:A:324:LEU:HD22	1:A:345:VAL:HG23	1.94	0.48
1:C:128:PHE:CZ	1:C:130:MET:HG3	2.49	0.48
1:B:483:PHE:HD2	1:B:484:LEU:HD13	1.79	0.48
1:A:53:LEU:N	1:A:53:LEU:HD23	2.29	0.47
1:D:111:VAL:HG21	1:D:234:ILE:CG2	2.44	0.47
1:E:189:ASN:ND2	1:E:192:SER:H	2.12	0.47
1:A:455:ASN:ND2	1:B:88:GLU:HG2	2.29	0.47
1:B:23:ARG:HB3	1:B:30:LEU:HD11	1.96	0.47
1:F:78:TYR:CZ	1:F:113:ARG:NH1	2.82	0.47
1:D:156:MET:HE1	1:D:173:TYR:HB2	1.96	0.47
1:E:103:ARG:CG	1:E:104:TYR:H	2.27	0.47
1:B:342:ILE:HD11	1:B:484:LEU:HD11	1.94	0.47
1:D:143:LEU:HD23	1:D:143:LEU:C	2.34	0.47
1:B:68:GLN:NE2	1:B:159:ARG:HH21	2.12	0.47
1:B:363:GLY:HA3	1:B:432:TYR:CZ	2.49	0.47
1:A:368:ASN:C	1:A:487:ALA:HB2	2.34	0.47
1:B:317:VAL:HG13	1:B:319:THR:HG22	1.95	0.47
1:D:146:ILE:HD11	1:D:157:PRO:HD3	1.95	0.47
1:A:52:THR:HA	1:A:138:VAL:O	2.14	0.47
1:C:374:HIS:O	1:C:420:ALA:HA	2.15	0.47
1:F:145:ASP:OD1	1:F:147:ARG:HG2	2.14	0.47
1:E:348:LEU:HD11	1:E:440:ARG:NH2	2.30	0.47
1:D:56:ASN:ND2	4:D:516:HOH:O	2.48	0.47
1:A:198:PHE:CD2	1:C:393:GLN:NE2	2.81	0.47
1:D:394:VAL:HG22	1:D:402:VAL:HG23	1.95	0.47
1:F:367:LYS:O	1:F:368:ASN:HB2	2.15	0.47
1:A:110:LYS:HG2	1:A:112:ASN:OD1	2.15	0.47
1:C:393:GLN:HA	1:C:403:PHE:O	2.14	0.47
1:B:232:LEU:HD22	1:B:232:LEU:HA	1.81	0.47
1:C:320:ALA:HA	3:C:499:GOL:H12	1.95	0.47
1:D:479:ASN:HA	1:D:480:PRO:HD3	1.69	0.47
1:A:161:TYR:HE1	4:A:517:HOH:O	1.98	0.47
1:B:326:ILE:HD12	1:B:362:HIS:HB2	1.97	0.47
1:D:195:LYS:HB2	1:E:393:GLN:HE22	1.80	0.47
1:E:67:PRO:HB3	1:E:356:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:VAL:HA	1:B:486:PRO:HD3	1.73	0.47
1:B:59:ARG:NH2	3:B:506:GOL:H31	2.30	0.46
1:C:320:ALA:HA	3:C:499:GOL:H2	1.97	0.46
1:A:479:ASN:HA	1:A:480:PRO:HD3	1.69	0.46
1:D:168:GLN:HG2	1:D:169:GLU:N	2.30	0.46
1:C:68:GLN:HE21	1:C:159:ARG:NH2	2.11	0.46
1:D:370:MET:HB2	1:D:423:ALA:O	2.14	0.46
1:D:107:ARG:O	1:D:107:ARG:HD2	2.16	0.46
1:D:143:LEU:HD13	1:D:435:PHE:HB3	1.97	0.46
1:F:12:LEU:CD2	1:F:39:LYS:HD3	2.45	0.46
1:F:323:ARG:HG2	1:F:324:LEU:N	2.30	0.46
1:E:344:THR:HG22	1:E:361:GLU:CG	2.44	0.46
1:A:378:ASN:HA	1:A:417:GLN:HE21	1.81	0.46
1:C:368:ASN:HD22	1:C:424:LYS:HE2	1.80	0.46
1:A:416:PRO:HB2	1:A:419:TYR:CD1	2.50	0.46
1:E:76:ASN:ND2	1:E:115:ARG:HA	2.29	0.46
1:D:389:ARG:HE	3:D:499:GOL:C1	2.28	0.46
1:B:196:ARG:HD2	1:B:207:ARG:HE	1.78	0.46
1:F:12:LEU:HD23	1:F:39:LYS:HD3	1.98	0.46
1:E:90:PHE:HD2	1:E:108:HIS:HE1	1.63	0.46
1:D:389:ARG:NH2	3:D:499:GOL:H12	2.26	0.46
1:D:203:PHE:CE2	1:D:213:LEU:HD21	2.51	0.46
1:C:353:LEU:HG	1:C:358:LEU:O	2.16	0.46
1:E:350:LEU:O	1:E:353:LEU:HB2	2.16	0.46
1:B:26:SER:CB	1:B:223:GLY:HA3	2.46	0.45
1:E:156:MET:HE3	1:E:157:PRO:HD2	1.98	0.45
1:F:401:THR:HG21	1:F:404:ASP:HB2	1.98	0.45
1:A:232:LEU:O	1:A:234:ILE:HG13	2.16	0.45
1:C:189:ASN:HD22	1:C:189:ASN:C	2.19	0.45
1:A:172:GLN:HG2	4:A:536:HOH:O	2.16	0.45
1:D:23:ARG:NH1	1:D:23:ARG:HG2	2.31	0.45
1:C:332:PRO:HG3	1:C:341:ARG:NH1	2.32	0.45
1:C:219:ASP:OD1	1:C:219:ASP:N	2.49	0.45
3:B:503:GOL:H11	4:B:529:HOH:O	2.16	0.45
1:D:389:ARG:HD2	1:D:406:GLU:OE2	2.17	0.45
1:A:69:GLU:HB2	1:A:358:LEU:HD13	1.97	0.45
1:A:8:ASN:HD21	1:B:156:MET:HG3	1.82	0.45
1:E:88:GLU:HB2	1:E:107:ARG:HD3	1.98	0.45
1:B:56:ASN:ND2	1:E:328:PRO:HB2	2.31	0.45
1:B:14:ARG:HG2	1:B:15:LEU:N	2.31	0.45
1:C:370:MET:HG3	1:C:485:VAL:CG1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:394:VAL:HG22	1:F:402:VAL:CG2	2.46	0.45
1:C:377:LEU:HD11	1:C:444:ALA:HB2	1.98	0.45
1:C:20:PRO:HG3	1:C:34:TRP:CH2	2.52	0.45
1:E:370:MET:CG	1:E:485:VAL:HG13	2.47	0.45
1:C:356:LEU:HD23	1:C:356:LEU:N	2.31	0.45
1:E:485:VAL:HA	1:E:486:PRO:HD3	1.82	0.45
1:D:427:SER:HA	3:D:499:GOL:H32	1.98	0.45
1:B:370:MET:CB	1:B:423:ALA:O	2.63	0.45
1:F:394:VAL:HG22	1:F:402:VAL:HG23	1.98	0.45
1:F:53:LEU:HD23	1:F:53:LEU:N	2.32	0.45
1:E:401:THR:CG2	1:E:404:ASP:HB2	2.46	0.45
1:A:196:ARG:O	1:A:200:GLU:HG3	2.16	0.45
1:D:107:ARG:CZ	1:D:107:ARG:H	2.30	0.45
1:A:65:ASN:HA	1:C:418:ASN:OD1	2.17	0.45
1:F:479:ASN:HA	1:F:480:PRO:HD3	1.70	0.45
1:A:452:VAL:O	1:A:456:LEU:HG	2.17	0.45
1:F:322:LEU:HD13	1:F:322:LEU:HA	1.76	0.44
1:F:52:THR:HA	1:F:138:VAL:O	2.17	0.44
1:C:389:ARG:HD2	1:C:406:GLU:OE2	2.17	0.44
1:D:317:VAL:O	1:D:317:VAL:HG13	2.17	0.44
1:D:36:PRO:HD2	1:D:173:TYR:CD1	2.52	0.44
1:B:90:PHE:C	1:B:90:PHE:CD1	2.90	0.44
1:C:53:LEU:HD22	1:C:225:ILE:CG2	2.47	0.44
1:B:479:ASN:HA	1:B:480:PRO:HD3	1.77	0.44
1:B:61:PRO:HB2	1:B:162:LEU:HD12	1.99	0.44
1:F:195[A]:LYS:O	1:F:198:PHE:HB2	2.16	0.44
1:D:130:MET:HE3	1:D:130:MET:HB3	1.69	0.44
1:F:58:LEU:HD13	1:F:60:ARG:HG2	1.98	0.44
1:A:401:THR:HB	1:B:183:GLN:NE2	2.32	0.44
1:C:350:LEU:HB3	1:C:353:LEU:HD22	1.99	0.44
1:F:344:THR:HG22	1:F:361:GLU:HG3	1.99	0.44
1:C:165:ASN:O	1:C:220:GLU:HB3	2.17	0.44
1:D:350:LEU:HB3	1:D:353:LEU:HD22	1.97	0.44
1:E:337:PRO:O	1:E:366:HIS:HE1	2.00	0.44
1:C:344:THR:HG22	1:C:361:GLU:CG	2.33	0.44
1:B:398:ASN:ND2	1:C:171:LEU:HG	2.31	0.44
1:A:332:PRO:HG3	1:A:341:ARG:CZ	2.48	0.44
1:D:218:GLU:HG3	1:D:222:LYS:HD2	2.00	0.44
1:A:203:PHE:CE2	1:A:213:LEU:HD21	2.53	0.44
1:C:143:LEU:HD13	1:C:435:PHE:HB2	1.99	0.44
1:F:200:GLU:OE2	1:F:207:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:GLN:HB3	1:F:168:GLN:HE21	1.68	0.44
1:F:110:LYS:HB2	1:F:110:LYS:HE2	1.75	0.44
1:F:335:TYR:CE2	1:F:337:PRO:HG3	2.53	0.44
1:D:168:GLN:HB3	1:D:168:GLN:HE21	1.49	0.44
1:A:105:ARG:O	1:A:105:ARG:HG3	2.18	0.44
1:C:130:MET:HE1	1:C:138:VAL:HG11	1.99	0.44
1:C:488:ARG:HD2	1:C:488:ARG:H	1.83	0.44
1:B:353:LEU:HD12	1:B:353:LEU:HA	1.84	0.44
1:E:235:ILE:N	1:E:235:ILE:HD13	2.33	0.44
1:D:36:PRO:HD2	1:D:173:TYR:CE1	2.53	0.44
1:D:165:ASN:O	1:D:220:GLU:HA	2.18	0.44
1:D:373:PRO:O	1:D:446:LEU:HB2	2.18	0.44
1:E:21:ASP:OD1	1:E:35:ASN:HB2	2.18	0.44
1:B:363:GLY:HA3	1:B:432:TYR:CE1	2.53	0.44
1:A:354:ARG:HG2	1:A:355:TRP:HD1	1.83	0.44
1:A:236:SER:HB2	1:A:237:PRO:CA	2.41	0.43
1:E:190:ILE:HD12	1:F:446:LEU:HD21	1.99	0.43
1:B:189:ASN:HD22	1:B:192:SER:H	1.66	0.43
1:F:55[B]:ARG:HD2	1:F:135:ASP:OD1	2.18	0.43
1:C:141:VAL:HG11	1:C:384:TYR:CE2	2.53	0.43
1:F:156:MET:HB3	1:F:156:MET:HE3	1.93	0.43
1:C:334:ILE:HG22	1:C:484:LEU:HD22	2.00	0.43
1:E:128:PHE:CZ	1:E:130:MET:HG3	2.53	0.43
1:A:83:PHE:CE2	1:A:322:LEU:HD21	2.53	0.43
1:D:401:THR:HG21	1:D:404:ASP:HB2	2.01	0.43
1:C:47:ALA:HA	4:C:507:HOH:O	2.18	0.43
1:D:67:PRO:CB	1:D:356:LEU:HD13	2.49	0.43
1:F:214:GLN:HE21	1:F:216:ARG:HE	1.64	0.43
1:F:189:ASN:HD22	1:F:191:PHE:N	2.16	0.43
1:D:195:LYS:HG2	2:D:497:SO4:O1	2.18	0.43
1:D:455:ASN:ND2	1:F:109:GLN:HG3	2.15	0.43
1:B:328:PRO:CG	3:B:504:GOL:H11	2.42	0.43
1:D:389:ARG:HE	3:D:499:GOL:H12	1.84	0.43
1:C:320:ALA:HA	3:C:499:GOL:C1	2.49	0.43
1:E:9:GLU:H	1:E:9:GLU:HG3	1.45	0.43
1:E:168:GLN:HB3	1:E:168:GLN:HE21	1.43	0.43
1:A:370:MET:HG3	1:A:485:VAL:CG1	2.49	0.43
1:D:445:ARG:CZ	1:D:482:LYS:HE3	2.49	0.43
1:F:365:LEU:HD13	1:F:370:MET:HA	2.00	0.43
1:A:324:LEU:HD22	1:A:345:VAL:CG2	2.49	0.43
1:B:68:GLN:HE21	1:B:159:ARG:HH21	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ASN:ND2	1:A:11:GLN:OE1	2.52	0.43
1:B:389:ARG:HG2	1:B:408:GLU:CB	2.49	0.43
1:B:54:GLN:HB3	3:B:507:GOL:H11	2.01	0.43
1:B:59:ARG:HH21	3:B:506:GOL:C3	2.32	0.43
1:C:220:GLU:CD	1:C:220:GLU:H	2.19	0.43
1:A:450:SER:N	4:A:529:HOH:O	2.42	0.43
1:A:449:THR:HB	1:A:482:LYS:HA	2.01	0.43
1:B:328:PRO:HA	3:B:504:GOL:O1	2.19	0.43
1:F:145:ASP:HB2	1:F:358:LEU:HD11	2.00	0.43
1:C:190:ILE:HD12	1:C:191:PHE:H	1.84	0.43
1:D:345:VAL:O	1:D:359:SER:HB2	2.18	0.43
1:D:381:SER:HB2	1:D:415:VAL:HB	2.01	0.43
1:F:370:MET:HG3	1:F:485:VAL:CG1	2.47	0.42
1:C:76:ASN:HD22	1:C:115:ARG:HB3	1.84	0.42
1:A:196:ARG:HB3	1:A:207:ARG:HH21	1.84	0.42
1:A:200:GLU:OE2	1:A:207:ARG:NH2	2.51	0.42
1:F:196:ARG:HD2	1:F:207:ARG:NH1	2.34	0.42
1:A:354:ARG:HG2	1:A:355:TRP:CD1	2.54	0.42
1:E:171:LEU:HG	1:F:398:ASN:ND2	2.34	0.42
1:A:417:GLN:O	1:A:418:ASN:HB2	2.18	0.42
1:C:20:PRO:HG3	1:C:34:TRP:CZ2	2.53	0.42
1:A:35:ASN:HA	1:A:36:PRO:HD2	1.84	0.42
1:F:81:MET:HA	1:F:127:VAL:O	2.19	0.42
1:B:15:LEU:HB2	1:B:403:PHE:HB2	2.01	0.42
1:E:162:LEU:CD2	1:E:190:ILE:HD11	2.49	0.42
1:A:111:VAL:HG21	1:A:234:ILE:HG21	2.01	0.42
1:E:109:GLN:HG3	1:F:455:ASN:ND2	2.33	0.42
1:A:113:ARG:NH2	4:A:543:HOH:O	2.52	0.42
1:A:82:VAL:HG11	1:C:452:VAL:HA	2.00	0.42
1:A:401:THR:HB	1:B:183:GLN:HE21	1.84	0.42
1:D:336:ASN:HA	1:D:337:PRO:HD2	1.89	0.42
1:D:328:PRO:CG	3:D:500:GOL:H31	2.30	0.42
1:B:437:THR:OG1	1:C:152:GLN:NE2	2.48	0.42
1:F:146:ILE:CD1	1:F:157:PRO:HD3	2.50	0.42
1:F:334:ILE:O	1:F:341:ARG:HA	2.20	0.42
1:C:394:VAL:HA	1:C:420:ALA:O	2.20	0.42
1:D:52:THR:HA	1:D:138:VAL:O	2.19	0.42
1:B:341:ARG:O	1:B:342:ILE:HD13	2.19	0.42
1:F:485:VAL:HA	1:F:486:PRO:HD3	1.84	0.42
1:A:105:ARG:N	1:A:106:ASP:CA	2.80	0.42
1:C:377:LEU:CD1	1:C:444:ALA:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:GLU:O	1:E:204:ASN:N	2.51	0.42
1:E:330:SER:OG	1:E:343:LYS:HG3	2.20	0.42
1:D:189:ASN:HD22	1:D:191:PHE:H	1.68	0.42
1:D:351:PRO:O	1:D:354:ARG:HG2	2.20	0.42
1:A:383:ILE:O	1:A:412:ALA:HA	2.20	0.42
1:F:190:ILE:HD12	1:F:191:PHE:N	2.35	0.42
1:E:219:ASP:OD2	1:E:220:GLU:N	2.53	0.42
1:C:234:ILE:HG22	1:C:235:ILE:N	2.33	0.42
1:F:7:GLN:HG2	1:F:8:ASN:ND2	2.34	0.42
1:C:157:PRO:HB2	1:C:170:PHE:CD2	2.54	0.42
1:C:189:ASN:HD22	1:C:192:SER:H	1.67	0.42
1:C:145:ASP:OD1	1:C:147:ARG:HG2	2.20	0.42
1:B:90:PHE:CB	1:B:106:ASP:O	2.68	0.42
1:B:53:LEU:HD22	1:B:225:ILE:CG2	2.49	0.42
1:B:220:GLU:HG3	1:B:220:GLU:O	2.19	0.42
1:A:109:GLN:HG3	1:C:455:ASN:ND2	2.34	0.42
1:F:214:GLN:HE22	1:F:216:ARG:HE	1.65	0.42
1:C:357:LYS:HD3	1:C:439:ASP:OD1	2.20	0.42
1:A:353:LEU:HG	1:A:358:LEU:O	2.19	0.41
1:B:66:ALA:HB1	1:B:67:PRO:HD2	2.01	0.41
1:E:90:PHE:HD2	1:E:108:HIS:CE1	2.38	0.41
1:C:152:GLN:HB3	1:C:152:GLN:HE21	1.62	0.41
1:B:465:PHE:CE1	1:C:163:ALA:HB2	2.56	0.41
1:C:196:ARG:HG2	1:C:214:GLN:HE22	1.84	0.41
1:A:105:ARG:O	1:A:105:ARG:CG	2.67	0.41
1:E:143:LEU:HD13	1:E:435:PHE:HB3	2.02	0.41
1:E:146:ILE:HD13	1:E:155:GLN:O	2.19	0.41
1:C:336:ASN:HA	1:C:337:PRO:HD3	1.79	0.41
1:F:408:GLU:HG2	4:F:509:HOH:O	2.20	0.41
1:D:219:ASP:N	1:D:219:ASP:OD1	2.48	0.41
1:F:115:ARG:NH1	3:F:498:GOL:O2	2.53	0.41
1:D:143:LEU:HD13	1:D:435:PHE:CB	2.50	0.41
1:E:394:VAL:HA	1:E:420:ALA:O	2.21	0.41
1:D:485:VAL:HA	1:D:486:PRO:HD3	1.95	0.41
1:E:86:CYS:HB2	1:E:109:GLN:NE2	2.35	0.41
1:B:317:VAL:CG1	1:B:319:THR:HG22	2.50	0.41
1:E:330:SER:HB2	1:E:343:LYS:HE2	2.02	0.41
1:E:141:VAL:HG11	1:E:384:TYR:CE2	2.55	0.41
1:A:80:GLY:O	1:A:128:PHE:HA	2.21	0.41
1:E:168:GLN:HG2	1:E:169:GLU:N	2.34	0.41
1:A:8:ASN:HD22	1:A:11:GLN:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ALA:HB2	1:B:157:PRO:HG3	2.03	0.41
1:B:427:SER:CB	3:B:505:GOL:H32	2.50	0.41
1:D:110:LYS:HG3	1:D:110:LYS:O	2.20	0.41
1:E:401:THR:HG21	1:E:404:ASP:HB2	2.02	0.41
1:F:366:HIS:O	1:F:425:SER:HB3	2.21	0.41
1:B:331:SER:HA	1:B:332:PRO:HD3	1.84	0.41
1:C:160:PHE:CD1	1:C:160:PHE:N	2.88	0.41
1:A:171:LEU:HD23	1:C:398:ASN:ND2	2.36	0.41
1:C:235:ILE:O	1:C:235:ILE:HG22	2.20	0.41
1:A:350:LEU:O	1:A:353:LEU:HB2	2.21	0.41
1:E:52:THR:HA	1:E:138:VAL:O	2.20	0.41
1:C:316:THR:HG22	1:C:355:TRP:HZ2	1.85	0.41
1:D:186:GLU:CG	1:D:187:GLY:H	2.34	0.41
1:E:146:ILE:HD11	1:E:157:PRO:HD3	2.03	0.41
1:E:202:ALA:O	1:F:479:ASN:ND2	2.52	0.41
1:F:377:LEU:HD11	1:F:444:ALA:HB2	2.01	0.41
1:E:160:PHE:CE2	1:F:397:CYS:HB3	2.55	0.41
1:E:76:ASN:ND2	1:E:116:GLU:H	2.19	0.41
1:B:156:MET:HE3	1:B:157:PRO:HD2	2.03	0.41
1:D:196:ARG:HG2	1:D:207:ARG:NE	2.36	0.41
1:C:143:LEU:HD13	1:C:435:PHE:CB	2.51	0.41
1:B:475:LEU:HD21	1:C:213:LEU:HD13	2.02	0.41
1:D:115:ARG:HH12	3:D:498:GOL:H31	1.86	0.41
1:B:83:PHE:HA	1:B:84:PRO:HD2	1.83	0.41
1:C:374:HIS:CE1	3:C:500:GOL:H2	2.56	0.41
1:E:69:GLU:HB2	1:E:358:LEU:HD13	2.02	0.41
1:D:130:MET:CE	1:D:138:VAL:HG11	2.46	0.41
1:F:391:ARG:NH1	1:F:404:ASP:OD1	2.53	0.41
1:B:90:PHE:HB2	1:B:106:ASP:O	2.21	0.41
1:D:446:LEU:HD12	1:D:446:LEU:HA	1.87	0.41
1:E:56:ASN:HA	1:E:132:ASN:O	2.21	0.41
1:D:465:PHE:CE1	1:F:163:ALA:HB2	2.56	0.41
1:C:205:VAL:HB	1:C:209:ILE:HD12	2.02	0.41
1:C:394:VAL:O	1:C:402:VAL:HG22	2.21	0.41
1:A:109:GLN:HG3	1:C:455:ASN:HD22	1.86	0.41
1:D:394:VAL:HG13	1:D:403:PHE:HB3	2.03	0.41
1:E:26:SER:HB2	1:E:222:LYS:O	2.21	0.41
1:C:88:GLU:HB3	1:C:89:THR:H	1.72	0.41
1:F:417:GLN:O	1:F:418:ASN:HB2	2.21	0.41
1:B:116:GLU:OE2	1:E:136:THR:OG1	2.29	0.41
1:D:168:GLN:HE22	1:E:398:ASN:HD21	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:LEU:HG	1:F:398:ASN:HD21	1.86	0.40
1:F:146:ILE:HD13	1:F:157:PRO:HD3	2.03	0.40
1:D:201:ASP:OD1	1:E:488:ARG:HD3	2.20	0.40
1:B:346:THR:HB	1:B:439:ASP:O	2.20	0.40
1:D:196:ARG:NH2	1:D:216:ARG:HH11	2.20	0.40
1:F:176:GLN:H	1:F:176:GLN:CD	2.24	0.40
1:D:367:LYS:O	1:D:368:ASN:HB2	2.21	0.40
1:D:196:ARG:HD2	1:D:211:ASP:OD1	2.20	0.40
1:E:113:ARG:NH2	1:E:133:ASP:OD2	2.54	0.40
1:B:417:GLN:O	1:B:418:ASN:HB2	2.21	0.40
1:A:474:GLN:HE21	1:A:478:ASN:ND2	2.19	0.40
1:C:485:VAL:HA	1:C:486:PRO:HD3	1.79	0.40
1:C:68:GLN:HB2	1:C:122:VAL:HB	2.03	0.40
1:A:452:VAL:HA	1:B:82:VAL:HG11	2.02	0.40
1:F:320:ALA:O	1:F:322:LEU:HD22	2.22	0.40
1:A:236:SER:CB	1:A:237:PRO:HA	2.40	0.40
1:B:389:ARG:HD3	3:B:505:GOL:C1	2.41	0.40
1:A:331:SER:HA	1:A:332:PRO:HD3	1.85	0.40
1:A:212:ARG:HG3	1:C:467:LEU:HD23	2.02	0.40
1:A:353:LEU:HA	1:A:353:LEU:HD12	1.94	0.40
1:C:350:LEU:O	1:C:353:LEU:HB2	2.22	0.40
1:D:189:ASN:HD21	1:D:191:PHE:HB2	1.87	0.40
1:D:53:LEU:HD22	1:D:225:ILE:HD13	2.04	0.40
1:C:367:LYS:HB2	1:C:428:ASP:HA	2.02	0.40
1:C:457:PRO:O	1:C:461:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	372/496 (75%)	350 (94%)	20 (5%)	2 (0%)	34 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	375/496 (76%)	356 (95%)	18 (5%)	1 (0%)	46	72
1	C	367/496 (74%)	341 (93%)	26 (7%)	0	100	100
1	D	368/496 (74%)	344 (94%)	24 (6%)	0	100	100
1	E	375/496 (76%)	353 (94%)	21 (6%)	1 (0%)	46	72
1	F	371/496 (75%)	353 (95%)	17 (5%)	1 (0%)	46	72
All	All	2228/2976 (75%)	2097 (94%)	126 (6%)	5 (0%)	52	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	236	SER
1	F	87	PRO
1	A	153	LEU
1	B	153	LEU
1	A	235	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/425 (76%)	298 (92%)	26 (8%)	15	29
1	B	327/425 (77%)	300 (92%)	27 (8%)	14	27
1	C	319/425 (75%)	287 (90%)	32 (10%)	9	18
1	D	320/425 (75%)	295 (92%)	25 (8%)	16	30
1	E	327/425 (77%)	294 (90%)	33 (10%)	9	17
1	F	323/425 (76%)	287 (89%)	36 (11%)	8	13
All	All	1940/2550 (76%)	1761 (91%)	179 (9%)	11	21

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU

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Mol	Chain	Res	Type
1	A	21	ASP
1	A	48	LEU
1	A	53	LEU
1	A	58	LEU
1	A	143	LEU
1	A	155	GLN
1	A	168	GLN
1	A	172	GLN
1	A	189	ASN
1	A	197	ASP
1	A	199	LEU
1	A	226	VAL
1	A	322	LEU
1	A	323	ARG
1	A	341	ARG
1	A	353	LEU
1	A	391	ARG
1	A	394	VAL
1	A	395	VAL
1	A	446	LEU
1	A	454	ASN
1	A	460	VAL
1	A	470	ASN
1	A	485	VAL
1	A	488	ARG
1	B	9	GLU
1	B	14	ARG
1	B	48	LEU
1	B	58	LEU
1	B	86	CYS
1	B	90	PHE
1	B	135	ASP
1	B	141	VAL
1	B	147	ARG
1	B	168	GLN
1	B	171	LEU
1	B	175	HIS
1	B	183	GLN
1	B	184	GLU
1	B	186	GLU
1	B	189	ASN
1	B	199	LEU

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Mol	Chain	Res	Type
1	B	232	LEU
1	B	322	LEU
1	B	353	LEU
1	B	371	PHE
1	B	394	VAL
1	B	446	LEU
1	B	459	ASP
1	B	484	LEU
1	B	485	VAL
1	B	488	ARG
1	C	23	ARG
1	C	48	LEU
1	C	55	ARG
1	C	58	LEU
1	C	110	LYS
1	C	111	VAL
1	C	115	ARG
1	C	135	ASP
1	C	168	GLN
1	C	171	LEU
1	C	172	GLN
1	C	189	ASN
1	C	199	LEU
1	C	317	VAL
1	C	318	CYS
1	C	322	LEU
1	C	323	ARG
1	C	324	LEU
1	C	353	LEU
1	C	356	LEU
1	C	371	PHE
1	C	391	ARG
1	C	394	VAL
1	C	429	ARG
1	C	443	ILE
1	C	446	LEU
1	C	449	THR
1	C	460	VAL
1	C	482	LYS
1	C	484	LEU
1	C	485	VAL
1	C	488	ARG

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Mol	Chain	Res	Type
1	D	14	ARG
1	D	23	ARG
1	D	48	LEU
1	D	53	LEU
1	D	58	LEU
1	D	88	GLU
1	D	107	ARG
1	D	113	ARG
1	D	115	ARG
1	D	141	VAL
1	D	142	SER
1	D	152	GLN
1	D	168	GLN
1	D	171	LEU
1	D	172	GLN
1	D	196	ARG
1	D	199	LEU
1	D	322	LEU
1	D	353	LEU
1	D	356	LEU
1	D	391	ARG
1	D	446	LEU
1	D	460	VAL
1	D	484	LEU
1	D	485	VAL
1	E	9	GLU
1	E	14	ARG
1	E	48	LEU
1	E	58	LEU
1	E	89	THR
1	E	90	PHE
1	E	103	ARG
1	E	107	ARG
1	E	110	LYS
1	E	111	VAL
1	E	113	ARG
1	E	135	ASP
1	E	141	VAL
1	E	168	GLN
1	E	171	LEU
1	E	176	GLN
1	E	189	ASN

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Mol	Chain	Res	Type
1	E	199	LEU
1	E	226	VAL
1	E	229	LYS
1	E	234	ILE
1	E	235	ILE
1	E	322	LEU
1	E	331	SER
1	E	353	LEU
1	E	364	SER
1	E	391	ARG
1	E	394	VAL
1	E	395	VAL
1	E	446	LEU
1	E	460	VAL
1	E	484	LEU
1	E	485	VAL
1	F	27	GLU
1	F	48	LEU
1	F	53	LEU
1	F	58	LEU
1	F	106	ASP
1	F	110	LYS
1	F	111	VAL
1	F	141	VAL
1	F	147	ARG
1	F	168	GLN
1	F	176	GLN
1	F	189	ASN
1	F	192	SER
1	F	199	LEU
1	F	213	LEU
1	F	221	GLU
1	F	226	VAL
1	F	317	VAL
1	F	322	LEU
1	F	323	ARG
1	F	344	THR
1	F	353	LEU
1	F	354	ARG
1	F	387	LYS
1	F	391	ARG
1	F	394	VAL

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Mol	Chain	Res	Type
1	F	395	VAL
1	F	414	THR
1	F	429	ARG
1	F	443	ILE
1	F	446	LEU
1	F	449	THR
1	F	460	VAL
1	F	484	LEU
1	F	485	VAL
1	F	488	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	11	GLN
1	A	22	ASN
1	A	37	ASN
1	A	68	GLN
1	A	108	HIS
1	A	152	GLN
1	A	155	GLN
1	A	168	GLN
1	A	172	GLN
1	A	174	GLN
1	A	189	ASN
1	A	214	GLN
1	A	217	ASN
1	A	366	HIS
1	A	368	ASN
1	A	374	HIS
1	A	398	ASN
1	A	400	ASN
1	A	455	ASN
1	A	474	GLN
1	B	22	ASN
1	B	38	ASN
1	B	40	GLN
1	B	56	ASN
1	B	68	GLN
1	B	76	ASN
1	B	108	HIS

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Mol	Chain	Res	Type
1	B	134	GLN
1	B	152	GLN
1	B	172	GLN
1	B	174	GLN
1	B	189	ASN
1	B	214	GLN
1	B	362	HIS
1	B	368	ASN
1	B	393	GLN
1	B	400	ASN
1	B	455	ASN
1	B	468	GLN
1	B	470	ASN
1	B	474	GLN
1	C	56	ASN
1	C	68	GLN
1	C	76	ASN
1	C	152	GLN
1	C	172	GLN
1	C	174	GLN
1	C	189	ASN
1	C	214	GLN
1	C	366	HIS
1	C	368	ASN
1	C	398	ASN
1	C	400	ASN
1	C	454	ASN
1	C	455	ASN
1	C	474	GLN
1	D	8	ASN
1	D	37	ASN
1	D	56	ASN
1	D	76	ASN
1	D	108	HIS
1	D	112	ASN
1	D	152	GLN
1	D	155	GLN
1	D	168	GLN
1	D	172	GLN
1	D	189	ASN
1	D	214	GLN
1	D	393	GLN

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Mol	Chain	Res	Type
1	D	400	ASN
1	D	454	ASN
1	D	455	ASN
1	E	37	ASN
1	E	56	ASN
1	E	68	GLN
1	E	76	ASN
1	E	108	HIS
1	E	112	ASN
1	E	152	GLN
1	E	168	GLN
1	E	172	GLN
1	E	174	GLN
1	E	176	GLN
1	E	189	ASN
1	E	214	GLN
1	E	217	ASN
1	E	362	HIS
1	E	368	ASN
1	E	398	ASN
1	E	400	ASN
1	E	455	ASN
1	E	468	GLN
1	F	7	GLN
1	F	8	ASN
1	F	68	GLN
1	F	108	HIS
1	F	152	GLN
1	F	155	GLN
1	F	175	HIS
1	F	176	GLN
1	F	189	ASN
1	F	214	GLN
1	F	217	ASN
1	F	368	ASN
1	F	398	ASN
1	F	400	ASN
1	F	455	ASN
1	F	468	GLN
1	F	474	GLN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

31 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	497	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	A	498	-	4,4,4	0.17	0	6,6,6	0.07	0
3	GOL	A	499	-	5,5,5	0.36	0	5,5,5	0.14	0
3	GOL	A	500	-	5,5,5	0.29	0	5,5,5	0.27	0
2	SO4	B	497	-	4,4,4	0.29	0	6,6,6	0.29	0
2	SO4	B	498	-	4,4,4	0.30	0	6,6,6	0.11	0
2	SO4	B	499	-	4,4,4	0.21	0	6,6,6	0.12	0
2	SO4	B	500	-	4,4,4	0.20	0	6,6,6	0.13	0
2	SO4	B	501	-	4,4,4	0.12	0	6,6,6	0.08	0
2	SO4	B	502	-	4,4,4	0.15	0	6,6,6	0.13	0
3	GOL	B	503	-	5,5,5	0.27	0	5,5,5	0.39	0
3	GOL	B	504	-	5,5,5	0.38	0	5,5,5	0.53	0
3	GOL	B	505	-	5,5,5	0.37	0	5,5,5	0.40	0
3	GOL	B	506	-	5,5,5	0.41	0	5,5,5	0.27	0
3	GOL	B	507	-	5,5,5	0.39	0	5,5,5	0.29	0
2	SO4	C	497	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	C	498	-	4,4,4	0.12	0	6,6,6	0.07	0
3	GOL	C	499	-	5,5,5	0.32	0	5,5,5	0.37	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	C	500	-	5,5,5	0.45	0	5,5,5	0.54	0
3	GOL	C	501	-	5,5,5	0.30	0	5,5,5	0.30	0
3	GOL	C	502	-	5,5,5	0.40	0	5,5,5	0.39	0
2	SO4	D	497	-	4,4,4	0.13	0	6,6,6	0.12	0
3	GOL	D	498	-	5,5,5	0.35	0	5,5,5	0.20	0
3	GOL	D	499	-	5,5,5	0.35	0	5,5,5	0.24	0
3	GOL	D	500	-	5,5,5	0.34	0	5,5,5	0.23	0
2	SO4	E	497	-	4,4,4	0.17	0	6,6,6	0.09	0
2	SO4	E	498	-	4,4,4	0.15	0	6,6,6	0.09	0
3	GOL	E	499	-	5,5,5	0.32	0	5,5,5	0.31	0
3	GOL	F	497	-	5,5,5	0.28	0	5,5,5	0.46	0
3	GOL	F	498	-	5,5,5	0.37	0	5,5,5	0.26	0
3	GOL	F	499	-	5,5,5	0.33	0	5,5,5	0.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	497	-	-	0/0/0/0	0/0/0/0
2	SO4	A	498	-	-	0/0/0/0	0/0/0/0
3	GOL	A	499	-	-	0/4/4/4	0/0/0/0
3	GOL	A	500	-	-	0/4/4/4	0/0/0/0
2	SO4	B	497	-	-	0/0/0/0	0/0/0/0
2	SO4	B	498	-	-	0/0/0/0	0/0/0/0
2	SO4	B	499	-	-	0/0/0/0	0/0/0/0
2	SO4	B	500	-	-	0/0/0/0	0/0/0/0
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	502	-	-	0/0/0/0	0/0/0/0
3	GOL	B	503	-	-	0/4/4/4	0/0/0/0
3	GOL	B	504	-	-	0/4/4/4	0/0/0/0
3	GOL	B	505	-	-	0/4/4/4	0/0/0/0
3	GOL	B	506	-	-	0/4/4/4	0/0/0/0
3	GOL	B	507	-	-	0/4/4/4	0/0/0/0
2	SO4	C	497	-	-	0/0/0/0	0/0/0/0
2	SO4	C	498	-	-	0/0/0/0	0/0/0/0
3	GOL	C	499	-	-	0/4/4/4	0/0/0/0
3	GOL	C	500	-	-	0/4/4/4	0/0/0/0
3	GOL	C	501	-	-	0/4/4/4	0/0/0/0
3	GOL	C	502	-	-	0/4/4/4	0/0/0/0
2	SO4	D	497	-	-	0/0/0/0	0/0/0/0
3	GOL	D	498	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	499	-	-	0/4/4/4	0/0/0/0
3	GOL	D	500	-	-	0/4/4/4	0/0/0/0
2	SO4	E	497	-	-	0/0/0/0	0/0/0/0
2	SO4	E	498	-	-	0/0/0/0	0/0/0/0
3	GOL	E	499	-	-	0/4/4/4	0/0/0/0
3	GOL	F	497	-	-	0/4/4/4	0/0/0/0
3	GOL	F	498	-	-	0/4/4/4	0/0/0/0
3	GOL	F	499	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	GOL	2	0
3	B	503	GOL	6	0
3	B	504	GOL	10	0
3	B	505	GOL	4	0
3	B	506	GOL	4	0
3	B	507	GOL	3	0
3	C	499	GOL	4	0
3	C	500	GOL	3	0
3	C	501	GOL	1	0
3	C	502	GOL	3	0
2	D	497	SO4	1	0
3	D	498	GOL	1	0
3	D	499	GOL	5	0
3	D	500	GOL	2	0
3	F	497	GOL	1	0
3	F	498	GOL	2	0
3	F	499	GOL	4	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	380/496 (76%)	-0.24	4 (1%) 82 79	20, 34, 69, 124	0
1	B	383/496 (77%)	-0.30	5 (1%) 79 75	18, 31, 66, 106	0
1	C	375/496 (75%)	-0.28	5 (1%) 79 75	20, 32, 60, 96	0
1	D	376/496 (75%)	-0.32	3 (0%) 87 85	18, 31, 60, 105	0
1	E	383/496 (77%)	-0.26	6 (1%) 74 69	18, 32, 62, 113	0
1	F	377/496 (76%)	-0.22	3 (0%) 87 85	22, 36, 68, 103	0
All	All	2274/2976 (76%)	-0.27	26 (1%) 82 79	18, 33, 65, 124	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	488	ARG	5.4
1	B	235	ILE	5.1
1	E	236	SER	4.9
1	A	237	PRO	4.8
1	B	236	SER	4.3
1	B	90	PHE	3.8
1	A	238	PRO	3.7
1	D	175	HIS	3.7
1	C	87	PRO	3.6
1	F	107	ARG	3.5
1	F	176	GLN	3.4
1	B	237	PRO	3.2
1	A	236	SER	3.2
1	E	90	PHE	3.1
1	A	316	THR	2.8
1	C	88	GLU	2.7
1	D	88	GLU	2.6
1	E	235	ILE	2.6
1	D	317	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	176	GLN	2.5
1	C	316	THR	2.5
1	E	238	PRO	2.5
1	F	235	ILE	2.3
1	C	229	LYS	2.1
1	C	235	ILE	2.0
1	E	8	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	B	506	6/6	0.93	0.23	5.56	13,28,31,34	0
3	GOL	B	504	6/6	0.95	0.23	4.64	37,38,41,43	0
3	GOL	C	500	6/6	0.97	0.27	4.07	34,37,39,44	0
3	GOL	C	499	6/6	0.90	0.30	3.32	37,54,64,64	0
3	GOL	B	503	6/6	0.90	0.21	1.88	37,43,47,48	0
3	GOL	A	500	6/6	0.93	0.22	1.55	45,51,57,60	0
3	GOL	B	507	6/6	0.91	0.22	1.33	35,43,51,59	0
3	GOL	B	505	6/6	0.91	0.18	1.21	31,42,42,64	0
2	SO4	A	497	5/5	0.98	0.16	0.39	46,50,66,74	0
3	GOL	E	499	6/6	0.91	0.18	0.19	30,43,48,57	0
3	GOL	D	500	6/6	0.87	0.14	-0.12	46,52,52,53	0
2	SO4	B	498	5/5	0.99	0.14	-0.23	28,29,33,35	0
2	SO4	B	499	5/5	0.98	0.13	-0.35	41,43,48,52	0
3	GOL	D	498	6/6	0.94	0.17	-0.45	42,51,57,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	497	5/5	0.99	0.13	-0.69	40,42,49,55	0
3	GOL	F	497	6/6	0.90	0.14	-0.77	43,56,59,61	0
3	GOL	C	502	6/6	0.95	0.14	-0.82	43,45,52,56	0
2	SO4	C	498	5/5	0.96	0.14	-0.97	52,55,67,68	0
2	SO4	D	497	5/5	0.96	0.15	-0.99	59,66,79,81	0
2	SO4	A	498	5/5	0.98	0.11	-1.00	64,66,74,78	0
2	SO4	E	498	5/5	0.95	0.15	-1.54	67,74,89,95	0
2	SO4	B	502	5/5	0.93	0.12	-1.64	63,70,84,86	0
3	GOL	F	498	6/6	0.94	0.11	-2.16	44,55,58,59	0
2	SO4	B	500	5/5	0.96	0.10	-2.39	46,56,68,70	0
3	GOL	C	501	6/6	0.94	0.11	-2.61	44,49,51,52	0
2	SO4	B	501	5/5	0.97	0.10	-2.69	46,52,66,66	0
3	GOL	A	499	6/6	0.96	0.13	-2.92	30,55,58,62	0
3	GOL	D	499	6/6	0.89	0.17	-	41,45,50,56	0
2	SO4	E	497	5/5	0.94	0.14	-	59,69,83,92	0
2	SO4	C	497	5/5	0.95	0.10	-	56,58,68,80	0
3	GOL	F	499	6/6	0.91	0.18	-	57,61,70,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.