



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2016 – 05:01 PM EDT

PDB ID : 4XGU
Title : Structure of C. elegans PCH-2
Authors : Ye, Q.; Corbett, K.D.
Deposited on : 2015-01-02
Resolution : 2.30 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027674
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) : rb-20027674

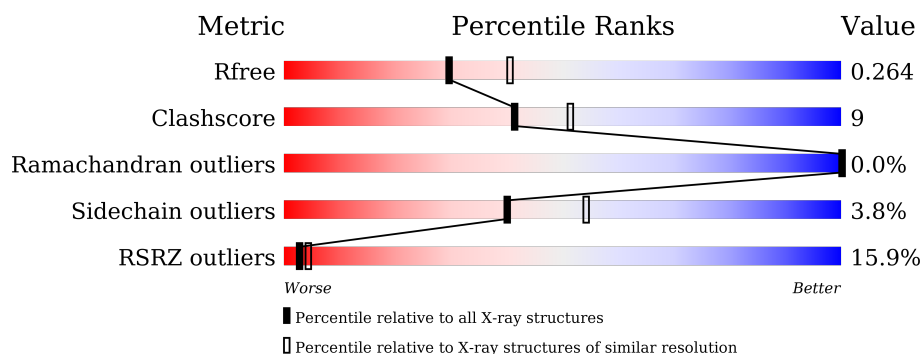
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 ≥ 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	424	<div> <div>18%</div> <div> <div>66%</div> <div>21%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	424	<div> <div>19%</div> <div> <div>67%</div> <div>21%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	424	<div> <div>13%</div> <div> <div>67%</div> <div>20%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	424	<div> <div>7%</div> <div> <div>75%</div> <div>13%</div> <div>•</div> <div>11%</div> </div> </div>
1	E	424	<div> <div>15%</div> <div> <div>70%</div> <div>18%</div> <div>•</div> <div>11%</div> </div> </div>
1	F	424	<div> <div>13%</div> <div> <div>66%</div> <div>21%</div> <div>•</div> <div>11%</div> </div> </div>

2 Entry composition [i](#)

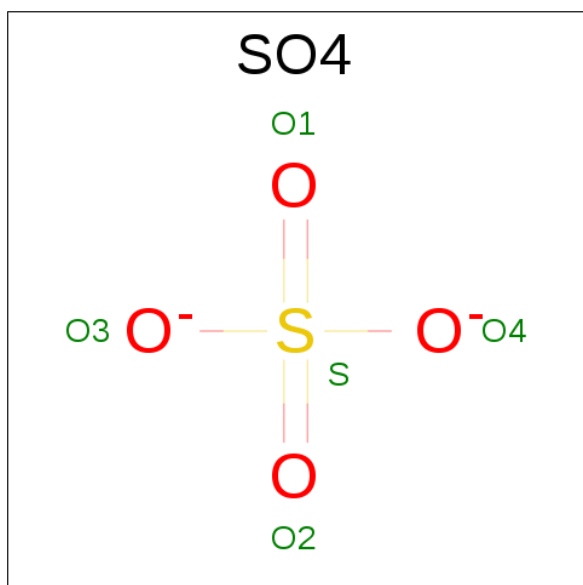
There are 4 unique types of molecules in this entry. The entry contains 17995 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative pachytene checkpoint protein 2.

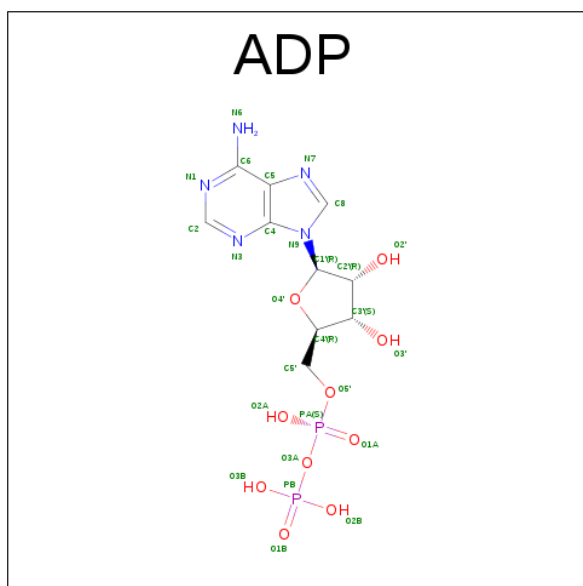
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2984	1885	516	565	18			
1	B	382	Total	C	N	O	S	0	0	0
			3020	1912	514	577	17			
1	C	374	Total	C	N	O	S	0	0	0
			2936	1853	505	561	17			
1	D	377	Total	C	N	O	S	0	0	0
			2981	1881	513	570	17			
1	E	379	Total	C	N	O	S	0	0	0
			2982	1884	511	570	17			
1	F	376	Total	C	N	O	S	0	0	0
			2948	1860	507	564	17			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0

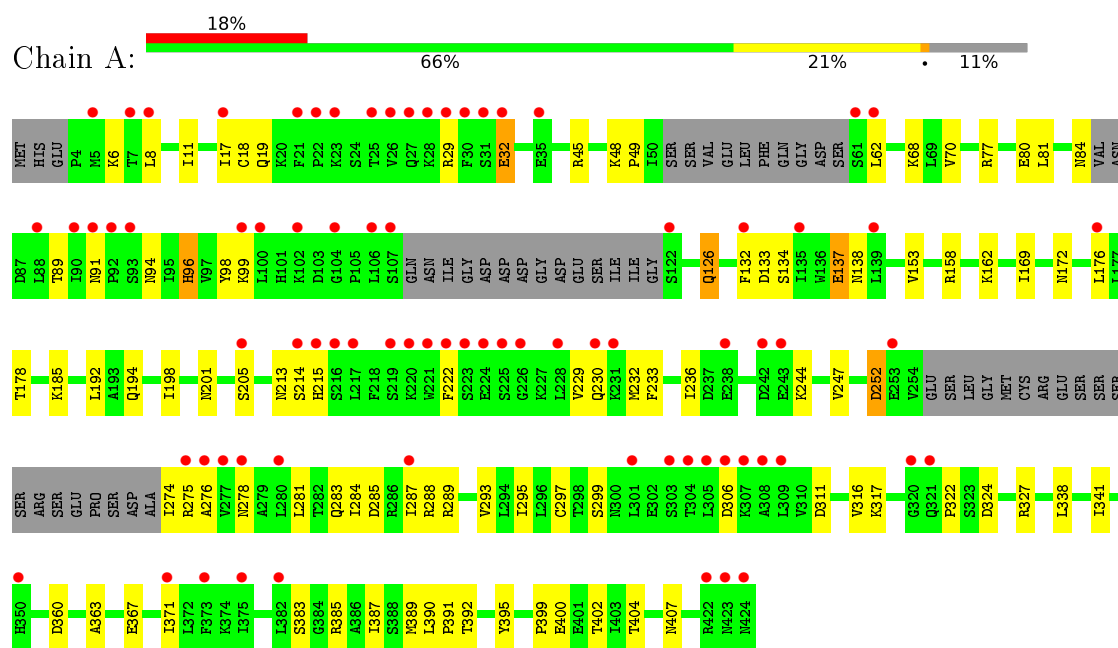
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	8	Total 8	O 8	0	0
4	C	13	Total 13	O 13	0	0
4	D	16	Total 16	O 16	0	0
4	E	11	Total 11	O 11	0	0
4	F	7	Total 7	O 7	0	0

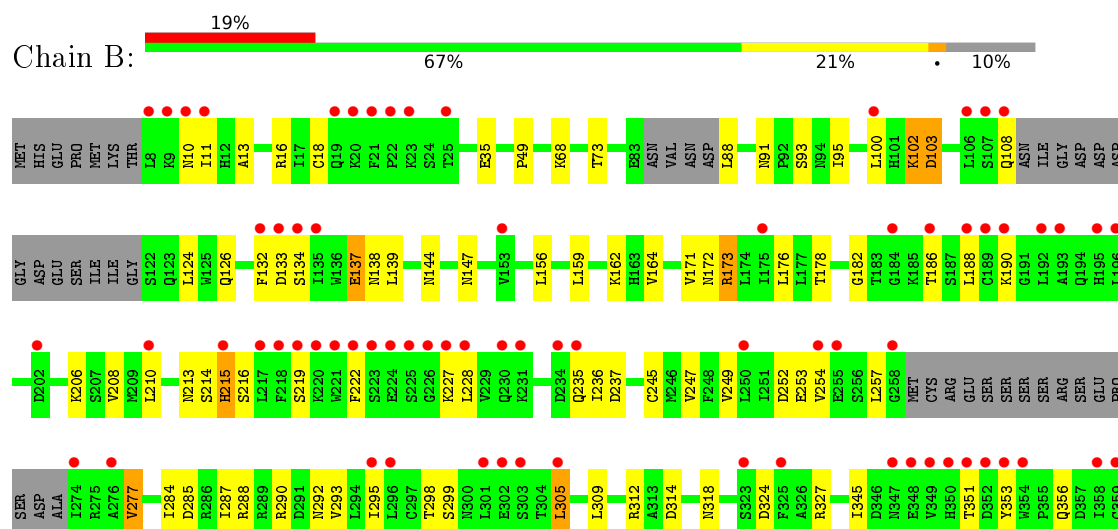
3 Residue-property plots

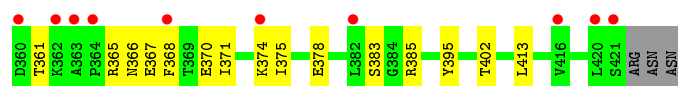
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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: Putative pachytene checkpoint protein 2

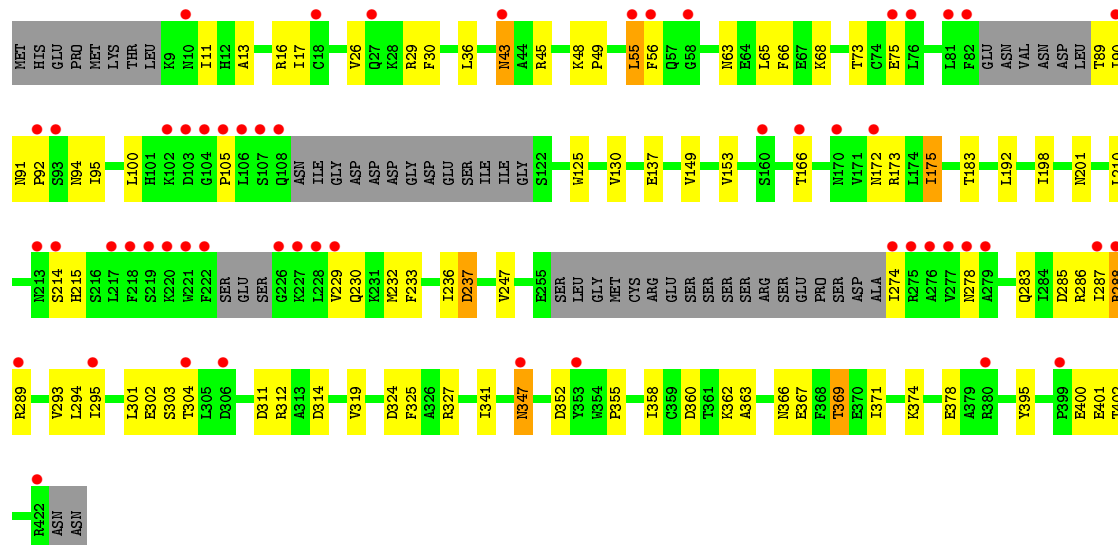


• Molecule 1: Putative pachytene checkpoint protein 2

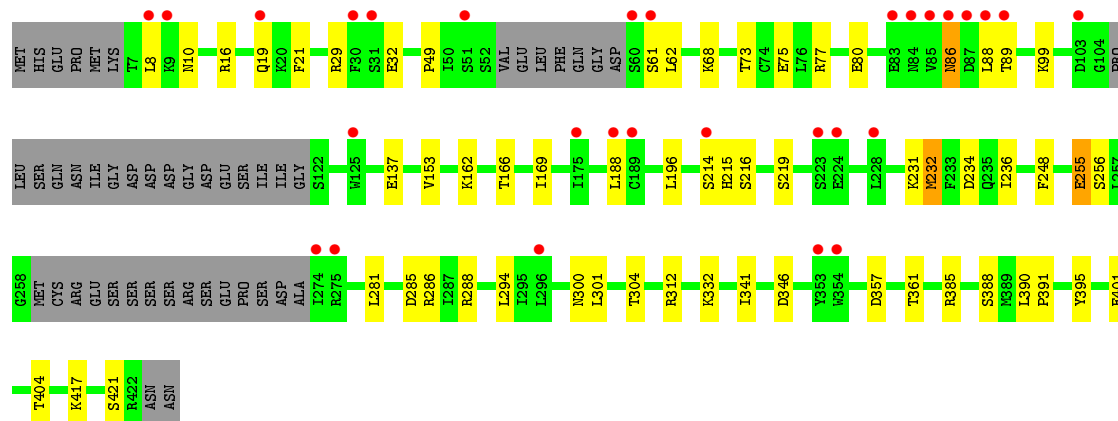
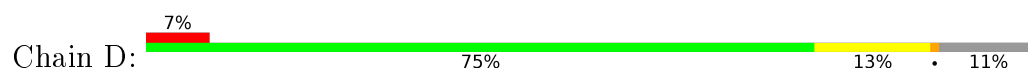




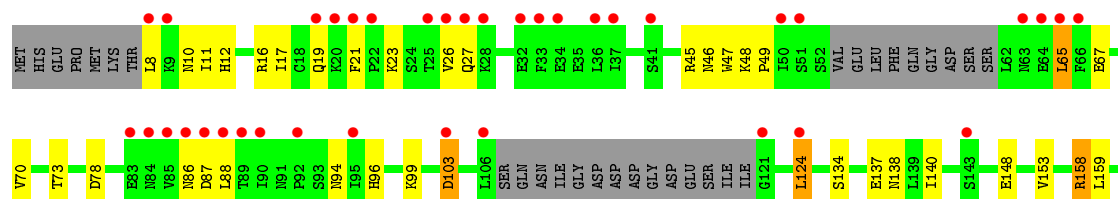
• Molecule 1: Putative pachytene checkpoint protein 2



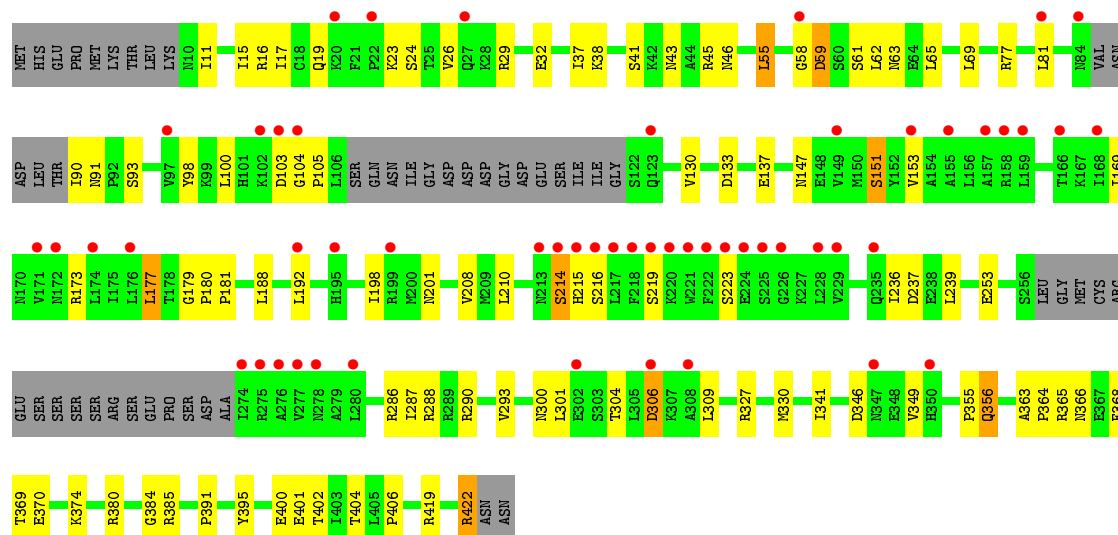
• Molecule 1: Putative pachytene checkpoint protein 2



• Molecule 1: Putative pachytene checkpoint protein 2



- Molecule 1: Putative pachytene checkpoint protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	126.71Å 240.97Å 197.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.36 – 2.30 39.36 – 2.30	Depositor EDS
% Data completeness (in resolution range)	71.8 (39.36-2.30) 71.8 (39.36-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.228 , 0.264 0.228 , 0.264	Depositor DCC
R_{free} test set	4881 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	60.0	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17995	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SO4, ADP

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	0.27	0/3028	0.41	0/4085
1	B	0.24	0/3066	0.40	0/4139
1	C	0.24	0/2978	0.41	0/4024
1	D	0.25	0/3025	0.41	0/4085
1	E	0.25	0/3027	0.44	0/4092
1	F	0.26	0/2992	0.41	0/4044
All	All	0.25	0/18116	0.41	0/24469

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	2984	0	3024	63	0
1	B	3020	0	3047	55	0
1	C	2936	0	2938	57	0
1	D	2981	0	3000	38	0
1	E	2982	0	2989	50	0
1	F	2948	0	2938	58	0
2	A	5	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	5	0	0	0	0
3	B	27	0	12	0	0
3	E	27	0	12	0	0
4	B	8	0	0	0	0
4	C	13	0	0	0	0
4	D	16	0	0	0	0
4	E	11	0	0	0	0
4	F	7	0	0	0	0
All	All	17995	0	17960	306	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 9.

All (306) 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:287:ILE:HG22	1:E:293:VAL:HG11	1.59	0.85
1:C:355:PRO:HA	1:C:369:THR:HG22	1.61	0.82
1:A:198:ILE:O	1:A:201:ASN:ND2	2.14	0.81
1:D:281:LEU:HB3	1:D:312:ARG:HH12	1.47	0.79
1:A:287:ILE:HG22	1:A:293:VAL:HG11	1.63	0.77
1:A:77:ARG:HB2	1:A:80:GLU:HG3	1.66	0.77
1:F:198:ILE:O	1:F:201:ASN:ND2	2.18	0.77
1:C:49:PRO:HD3	1:C:137:GLU:HG2	1.67	0.76
1:C:17:ILE:HD13	1:C:26:VAL:HG21	1.68	0.75
1:A:176:LEU:HD21	1:A:316:VAL:HG12	1.69	0.73
1:E:49:PRO:HB3	1:E:70:VAL:HG22	1.68	0.73
1:A:222:PHE:HE1	1:A:229:VAL:HG21	1.52	0.72
1:E:11:ILE:HG12	1:E:73:THR:HB	1.71	0.72
1:C:324:ASP:OD1	1:C:327:ARG:NH2	2.22	0.71
1:D:73:THR:HG22	1:D:75:GLU:H	1.55	0.71
1:D:19:GLN:HA	1:D:99:LYS:HD2	1.73	0.71
1:C:301:LEU:HD13	1:C:304:THR:HB	1.72	0.70
1:B:134:SER:O	1:B:138:ASN:ND2	2.24	0.69
1:C:153:VAL:HG22	1:C:175:ILE:HD12	1.73	0.69
1:B:49:PRO:HD3	1:B:137:GLU:HG2	1.75	0.69
1:E:16:ARG:HG2	1:E:67:GLU:HB2	1.74	0.69
1:F:29:ARG:HH12	1:F:61:SER:HB2	1.58	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:ARG:HB2	1:E:48:LYS:HB2	1.76	0.68
1:B:385:ARG:NH2	1:C:311:ASP:O	2.26	0.67
1:A:49:PRO:HD3	1:A:137:GLU:HG2	1.75	0.67
1:B:249:VAL:HB	1:B:295:ILE:HG22	1.75	0.67
1:B:16:ARG:NH2	1:B:133:ASP:OD2	2.26	0.67
1:C:153:VAL:HG21	1:C:192:LEU:HD21	1.76	0.67
1:A:8:LEU:HB3	1:A:11:ILE:HD11	1.76	0.66
1:C:283:GLN:OE1	1:C:286:ARG:NH1	2.28	0.66
1:E:17:ILE:HD13	1:E:26:VAL:HG11	1.77	0.66
1:F:404:THR:HG22	1:F:406:PRO:HD2	1.77	0.65
1:E:134:SER:O	1:E:138:ASN:ND2	2.29	0.65
1:A:45:ARG:HH22	1:A:360:ASP:HB2	1.62	0.65
1:C:17:ILE:HD11	1:C:26:VAL:HG11	1.78	0.64
1:B:237:ASP:OD1	1:B:290:ARG:NH2	2.30	0.64
1:F:173:ARG:NH1	1:F:288:ARG:O	2.30	0.64
1:C:13:ALA:HB3	1:C:95:ILE:HG13	1.80	0.63
1:D:49:PRO:HD3	1:D:137:GLU:HG2	1.80	0.63
1:D:401:GLU:OE1	1:E:158:ARG:NH2	2.32	0.62
1:C:91:ASN:HB2	1:C:94:ASN:HB2	1.82	0.62
1:B:13:ALA:HB3	1:B:95:ILE:HG22	1.81	0.62
1:E:96:HIS:ND1	1:E:201:ASN:OD1	2.27	0.61
1:A:324:ASP:OD1	1:A:327:ARG:NH1	2.32	0.61
1:D:388:SER:OG	1:E:170:ASN:ND2	2.33	0.61
1:D:385:ARG:NH2	1:E:311:ASP:O	2.33	0.61
1:A:132:PHE:HB3	1:A:194:GLN:HB2	1.83	0.61
1:D:234:ASP:OD1	1:D:286:ARG:NH2	2.34	0.61
1:A:400:GLU:OE2	1:A:400:GLU:N	2.34	0.61
1:C:166:THR:HG21	1:C:289:ARG:HH12	1.66	0.60
1:F:15:ILE:HD11	1:F:37:ILE:HD11	1.84	0.60
1:A:134:SER:O	1:A:138:ASN:ND2	2.33	0.60
1:B:178:THR:OG1	1:B:318:ASN:ND2	2.34	0.60
1:C:366:ASN:HB2	1:C:369:THR:HG23	1.84	0.60
1:F:17:ILE:HD13	1:F:26:VAL:HG21	1.84	0.59
1:F:58:GLY:HA2	1:F:59:ASP:HB2	1.83	0.59
1:A:19:GLN:HA	1:A:99:LYS:HD2	1.84	0.59
1:D:32:GLU:HB3	1:D:62:LEU:HD21	1.84	0.59
1:B:172:ASN:OD1	1:B:288:ARG:NH2	2.36	0.58
1:A:222:PHE:CE1	1:A:229:VAL:HG21	2.38	0.58
1:C:36:LEU:HD11	1:C:55:LEU:HD11	1.85	0.58
1:E:12:HIS:HA	1:E:94:ASN:HB3	1.86	0.58
1:C:285:ASP:OD1	1:C:312:ARG:NH1	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:ASP:OD1	1:D:288:ARG:NH1	2.36	0.58
1:E:19:GLN:HA	1:E:99:LYS:HE2	1.84	0.58
1:C:183:THR:HB	1:C:319:VAL:HG11	1.85	0.57
1:D:255:GLU:OE2	1:D:300:ASN:ND2	2.37	0.57
1:E:103:ASP:OD1	1:E:103:ASP:N	2.37	0.57
1:E:23:LYS:O	1:E:27:GLN:HG3	2.04	0.57
1:A:233:PHE:HD1	1:A:236:ILE:HD12	1.69	0.57
1:B:351:THR:O	1:B:356:GLN:NE2	2.37	0.57
1:C:347:ASN:OD1	1:C:347:ASN:N	2.37	0.56
1:A:252:ASP:N	1:A:252:ASP:OD1	2.38	0.56
1:A:322:PRO:O	1:A:327:ARG:NH2	2.38	0.56
1:A:399:PRO:O	1:B:10:ASN:HB2	2.05	0.56
1:F:356:GLN:H	1:F:369:THR:HG22	1.70	0.56
1:A:247:VAL:HB	1:A:293:VAL:HG22	1.88	0.56
1:B:324:ASP:OD1	1:B:327:ARG:NH2	2.36	0.56
1:B:126:GLN:HE22	1:B:206:LYS:HE3	1.71	0.56
1:F:29:ARG:HD3	1:F:65:LEU:HD11	1.87	0.56
1:E:391:PRO:HG2	1:F:169:ILE:HG23	1.87	0.56
1:E:140:ILE:HG21	1:E:329:SER:HB2	1.87	0.56
1:F:32:GLU:HB3	1:F:62:LEU:HD11	1.88	0.56
1:E:163:HIS:ND1	1:E:291:ASP:OD2	2.40	0.55
1:F:45:ARG:HG2	1:F:81:LEU:HD23	1.88	0.55
1:F:287:ILE:HG22	1:F:293:VAL:HG21	1.88	0.55
1:E:185:LYS:NZ	1:E:300:ASN:OD1	2.33	0.55
1:A:311:ASP:OD1	1:F:385:ARG:NH2	2.40	0.55
1:B:210:LEU:HD13	1:B:236:ILE:HG12	1.89	0.55
1:C:230:GLN:HA	1:C:283:GLN:HE21	1.71	0.55
1:C:352:ASP:O	1:C:366:ASN:ND2	2.40	0.55
1:E:285:ASP:OD1	1:E:288:ARG:NH1	2.39	0.54
1:A:178:THR:HG22	1:A:299:SER:HB3	1.88	0.54
1:C:43:ASN:OD1	1:C:43:ASN:N	2.40	0.54
1:F:237:ASP:OD2	1:F:286:ARG:NH1	2.40	0.54
1:C:17:ILE:CD1	1:C:26:VAL:HG11	2.37	0.54
1:E:86:ASN:OD1	1:E:87:ASP:N	2.36	0.54
1:A:172:ASN:OD1	1:A:288:ARG:NH2	2.40	0.54
1:B:285:ASP:OD1	1:B:312:ARG:NE	2.33	0.54
1:C:360:ASP:HB3	1:C:363:ALA:HB2	1.89	0.54
1:B:247:VAL:HG22	1:B:293:VAL:HG22	1.89	0.54
1:D:346:ASP:OD2	1:D:404:THR:OG1	2.25	0.53
1:C:237:ASP:OD2	1:C:286:ARG:NH2	2.41	0.53
1:A:45:ARG:HB2	1:A:48:LYS:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LEU:HD13	1:B:188:LEU:HD23	1.90	0.53
1:E:153:VAL:HG12	1:E:196:LEU:HD11	1.89	0.53
1:F:219:SER:O	1:F:223:SER:N	2.40	0.53
1:F:38:LYS:O	1:F:41:SER:OG	2.21	0.53
1:F:43:ASN:OD1	1:F:43:ASN:N	2.42	0.53
1:F:147:ASN:O	1:F:151:SER:OG	2.27	0.52
1:F:90:ILE:HG12	1:F:91:ASN:H	1.74	0.52
1:C:287:ILE:HG22	1:C:293:VAL:HG21	1.90	0.52
1:A:400:GLU:HG2	1:A:402:THR:O	2.10	0.52
1:C:302:GLU:OE2	1:C:302:GLU:N	2.41	0.52
1:A:389:MET:O	1:A:392:THR:HG22	2.10	0.52
1:C:210:LEU:HD22	1:C:236:ILE:HD11	1.91	0.52
1:F:419:ARG:NH2	1:F:422:ARG:O	2.43	0.52
1:B:144:ASN:HD21	1:B:147:ASN:HD22	1.58	0.52
1:C:173:ARG:HB2	1:C:294:LEU:HD23	1.92	0.52
1:F:19:GLN:OE1	1:F:19:GLN:N	2.42	0.52
1:A:96:HIS:HB2	1:A:201:ASN:HD21	1.76	0.51
1:E:237:ASP:OD1	1:E:290:ARG:NE	2.42	0.51
1:F:366:ASN:HB2	1:F:369:THR:HG23	1.91	0.51
1:F:301:LEU:HD13	1:F:304:THR:HB	1.92	0.51
1:E:148:GLU:OE1	1:E:317:LYS:NZ	2.41	0.51
1:E:249:VAL:HB	1:E:295:ILE:HG22	1.92	0.51
1:F:91:ASN:HD21	1:F:93:SER:HB2	1.75	0.51
1:E:174:LEU:HD12	1:E:295:ILE:HD11	1.93	0.50
1:E:21:PHE:HE2	1:E:65:LEU:HB2	1.77	0.50
1:A:213:ASN:ND2	1:A:252:ASP:O	2.44	0.50
1:D:301:LEU:HD13	1:D:304:THR:HG23	1.94	0.50
1:D:153:VAL:HG12	1:D:196:LEU:HD11	1.93	0.50
1:D:332:LYS:NZ	1:D:357:ASP:OD1	2.45	0.50
1:F:210:LEU:HD22	1:F:236:ILE:HD11	1.93	0.50
1:E:159:LEU:O	1:E:164:VAL:HG23	2.12	0.49
1:B:216:SER:OG	1:B:253:GLU:OE1	2.30	0.49
1:C:100:LEU:HD13	1:C:130:VAL:HA	1.95	0.49
1:C:29:ARG:HH11	1:C:65:LEU:HD11	1.76	0.49
1:A:233:PHE:CD2	1:A:283:GLN:HB3	2.48	0.49
1:C:105:PRO:HB3	1:C:125:TRP:CZ3	2.47	0.49
1:B:16:ARG:NH2	1:B:68:LYS:HD3	2.27	0.49
1:E:254:VAL:HG11	1:E:309:LEU:HD22	1.95	0.49
1:F:15:ILE:HG12	1:F:69:LEU:HD13	1.94	0.49
1:A:98:TYR:HB3	1:A:198:ILE:HG23	1.95	0.48
1:B:103:ASP:OD1	1:B:103:ASP:N	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:ASN:OD1	1:D:86:ASN:N	2.46	0.48
1:F:330:MET:HE1	1:F:384:GLY:HA2	1.95	0.48
1:A:385:ARG:O	1:A:389:MET:HG2	2.13	0.48
1:B:132:PHE:CZ	1:B:190:LYS:HD2	2.48	0.48
1:F:355:PRO:HA	1:F:369:THR:HG22	1.95	0.48
1:A:284:ILE:HG13	1:A:295:ILE:HD13	1.95	0.48
1:B:91:ASN:ND2	1:B:93:SER:HB3	2.28	0.48
1:A:6:LYS:HD2	1:A:84:ASN:HB2	1.94	0.48
1:B:213:ASN:ND2	1:B:252:ASP:O	2.43	0.48
1:A:68:LYS:NZ	1:A:133:ASP:OD1	2.45	0.48
1:C:45:ARG:HB2	1:C:48:LYS:HB2	1.96	0.48
1:B:156:LEU:HD22	1:B:171:VAL:HG13	1.95	0.48
1:A:172:ASN:HA	1:A:288:ARG:HH21	1.79	0.47
1:A:338:LEU:HA	1:A:341:ILE:HD12	1.95	0.47
1:B:361:THR:HG22	1:B:365:ARG:HH21	1.80	0.47
1:E:153:VAL:HG21	1:E:192:LEU:HD21	1.97	0.47
1:A:360:ASP:OD1	1:A:363:ALA:N	2.46	0.47
1:C:11:ILE:HG12	1:C:73:THR:HB	1.96	0.47
1:D:77:ARG:HB2	1:D:80:GLU:HB2	1.97	0.47
1:E:247:VAL:HB	1:E:293:VAL:HG22	1.97	0.47
1:B:284:ILE:O	1:B:288:ARG:HG2	2.14	0.47
1:D:214:SER:HA	1:D:215:HIS:HA	1.51	0.47
1:F:11:ILE:HG13	1:F:90:ILE:HG13	1.96	0.47
1:B:345:ILE:HB	1:B:402:THR:HG21	1.97	0.46
1:E:285:ASP:OD2	1:E:312:ARG:NH1	2.48	0.46
1:F:306:ASP:N	1:F:306:ASP:OD1	2.47	0.46
1:A:205:SER:HB3	1:A:244:LYS:HE3	1.97	0.46
1:C:247:VAL:HB	1:C:293:VAL:HG12	1.95	0.46
1:F:214:SER:HA	1:F:215:HIS:HA	1.55	0.46
1:F:59:ASP:OD1	1:F:59:ASP:N	2.49	0.46
1:B:11:ILE:HG23	1:B:73:THR:HB	1.98	0.46
1:A:383:SER:O	1:A:387:ILE:HG13	2.16	0.46
1:C:29:ARG:HD2	1:C:65:LEU:HD11	1.97	0.46
1:F:346:ASP:OD1	1:F:349:VAL:N	2.39	0.46
1:C:400:GLU:C	1:C:402:THR:H	2.19	0.46
1:E:8:LEU:HD21	1:E:11:ILE:HG13	1.98	0.46
1:B:366:ASN:HD22	1:B:366:ASN:H	1.63	0.46
1:A:317:LYS:HD3	1:A:317:LYS:HA	1.73	0.45
1:F:17:ILE:HD11	1:F:26:VAL:HG11	1.97	0.45
1:B:182:GLY:HA3	1:B:383:SER:HB2	1.97	0.45
1:E:360:ASP:O	1:E:362:LYS:HG3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:LEU:HD21	1:B:305:LEU:HD21	1.98	0.45
1:E:285:ASP:OD1	1:E:312:ARG:HD3	2.16	0.45
1:F:16:ARG:HB2	1:F:98:TYR:CZ	2.51	0.45
1:E:21:PHE:CE2	1:E:65:LEU:HB2	2.52	0.45
1:F:100:LEU:HD13	1:F:130:VAL:HA	1.98	0.45
1:F:214:SER:OG	1:F:214:SER:O	2.34	0.45
1:B:178:THR:HG22	1:B:299:SER:HB3	1.98	0.45
1:D:166:THR:HA	1:D:169:ILE:O	2.16	0.45
1:A:281:LEU:O	1:A:284:ILE:HG22	2.16	0.45
1:D:196:LEU:HD23	1:D:196:LEU:HA	1.84	0.45
1:A:341:ILE:HD11	1:B:164:VAL:HG22	1.99	0.45
1:B:124:LEU:HD11	1:B:208:VAL:HB	1.98	0.45
1:B:214:SER:HA	1:B:215:HIS:HA	1.59	0.45
1:C:173:ARG:N	1:C:314:ASP:OD2	2.50	0.45
1:C:233:PHE:HA	1:C:236:ILE:HD12	1.99	0.45
1:E:23:LYS:HD2	1:E:23:LYS:H	1.82	0.45
1:E:281:LEU:HD13	1:E:312:ARG:NH2	2.31	0.45
1:A:32:GLU:H	1:A:32:GLU:HG2	1.42	0.45
1:F:327:ARG:CZ	1:F:380:ARG:HA	2.47	0.45
1:B:254:VAL:HG11	1:B:309:LEU:HD22	1.98	0.44
1:E:185:LYS:NZ	1:E:300:ASN:HA	2.32	0.44
1:E:214:SER:HA	1:E:215:HIS:HA	1.56	0.44
1:A:68:LYS:NZ	1:A:137:GLU:OE2	2.50	0.44
1:F:91:ASN:ND2	1:F:93:SER:HB2	2.32	0.44
1:A:367:GLU:O	1:A:371:ILE:HG13	2.18	0.44
1:D:341:ILE:HD13	1:E:164:VAL:HG22	1.98	0.44
1:B:159:LEU:O	1:B:164:VAL:HG23	2.17	0.44
1:B:245:CYS:O	1:B:292:ASN:ND2	2.50	0.44
1:C:288:ARG:HG3	1:C:295:ILE:HD12	1.99	0.44
1:D:255:GLU:OE1	1:D:300:ASN:N	2.32	0.44
1:B:91:ASN:HD21	1:B:93:SER:HB3	1.82	0.44
1:C:400:GLU:HA	1:D:10:ASN:ND2	2.32	0.44
1:B:366:ASN:O	1:B:370:GLU:N	2.47	0.44
1:D:417:LYS:O	1:D:421:SER:OG	2.32	0.44
1:B:108:GLN:HG2	1:B:235:GLN:HE22	1.83	0.43
1:C:374:LYS:O	1:C:378:GLU:HG2	2.18	0.43
1:D:216:SER:O	1:D:219:SER:OG	2.32	0.43
1:E:159:LEU:HD22	1:E:164:VAL:HG21	1.98	0.43
1:F:153:VAL:HG21	1:F:192:LEU:HD21	1.98	0.43
1:F:179:GLY:O	1:F:300:ASN:HA	2.17	0.43
1:F:400:GLU:C	1:F:402:THR:H	2.21	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ILE:O	1:C:278:ASN:ND2	2.51	0.43
1:C:30:PHE:HZ	1:C:92:PRO:HA	1.83	0.43
1:D:21:PHE:HD1	1:D:21:PHE:N	2.16	0.43
1:E:158:ARG:O	1:E:162:LYS:HG2	2.18	0.43
1:B:375:ILE:HG12	1:B:413:LEU:HD13	2.01	0.43
1:C:73:THR:OG1	1:C:75:GLU:HG2	2.18	0.43
1:E:88:LEU:HA	1:E:88:LEU:HD12	1.85	0.43
1:B:178:THR:HG21	1:B:305:LEU:HD11	2.01	0.43
1:C:232:MET:O	1:C:236:ILE:HG13	2.18	0.43
1:F:55:LEU:O	1:F:63:ASN:ND2	2.51	0.43
1:A:169:ILE:HG23	1:F:391:PRO:HG2	2.00	0.43
1:D:21:PHE:N	1:D:21:PHE:CD1	2.86	0.43
1:A:126:GLN:HE21	1:A:126:GLN:HB3	1.55	0.43
1:A:153:VAL:HG21	1:A:192:LEU:HD21	2.01	0.43
1:A:275:ARG:HA	1:A:278:ASN:HD22	1.84	0.43
1:A:176:LEU:HA	1:A:297:CYS:O	2.17	0.43
1:D:21:PHE:O	1:D:99:LYS:NZ	2.51	0.43
1:E:317:LYS:HD3	1:E:317:LYS:HA	1.79	0.43
1:F:216:SER:N	1:F:253:GLU:OE1	2.51	0.43
1:A:274:ILE:HG22	1:A:276:ALA:H	1.84	0.43
1:A:45:ARG:HD3	1:A:81:LEU:HG	2.00	0.43
1:B:11:ILE:HD12	1:B:88:LEU:HD11	2.00	0.43
1:C:198:ILE:O	1:C:201:ASN:HB2	2.18	0.43
1:C:367:GLU:O	1:C:371:ILE:HG13	2.19	0.42
1:F:177:LEU:HD11	1:F:188:LEU:HD23	2.01	0.42
1:F:208:VAL:HG11	1:F:239:LEU:HD13	2.01	0.42
1:B:374:LYS:O	1:B:378:GLU:HG2	2.19	0.42
1:C:16:ARG:HH21	1:C:68:LYS:HE2	1.84	0.42
1:A:17:ILE:HG22	1:A:18:CYS:O	2.19	0.42
1:A:91:ASN:HD22	1:A:94:ASN:ND2	2.18	0.42
1:D:390:LEU:N	1:D:391:PRO:HD2	2.35	0.42
1:A:185:LYS:HG3	2:A:501:SO4:O3	2.20	0.42
1:C:229:VAL:O	1:C:233:PHE:HD2	2.01	0.42
1:B:222:PHE:CE2	1:B:277:VAL:HG12	2.55	0.42
1:F:370:GLU:O	1:F:374:LYS:HG2	2.18	0.42
1:A:404:THR:HG22	1:A:407:ASN:HB2	2.02	0.42
1:E:46:ASN:HB3	1:E:78:ASP:O	2.19	0.42
1:A:158:ARG:NH2	1:F:401:GLU:HG3	2.34	0.42
1:D:16:ARG:NH2	1:D:68:LYS:HE3	2.35	0.42
1:E:124:LEU:HD12	1:E:210:LEU:HD21	2.01	0.42
1:E:47:TRP:HH2	1:E:199:ARG:HH21	1.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:TRP:O	1:E:225:SER:N	2.53	0.42
1:A:285:ASP:O	1:A:289:ARG:HG3	2.20	0.42
1:A:390:LEU:N	1:A:391:PRO:HD2	2.34	0.42
1:B:287:ILE:CG2	1:B:293:VAL:HG11	2.50	0.42
1:C:341:ILE:HG23	1:D:162:LYS:HB3	2.01	0.42
1:D:255:GLU:HG2	1:D:256:SER:N	2.34	0.42
1:D:62:LEU:H	1:D:62:LEU:HD12	1.85	0.42
1:F:46:ASN:ND2	1:F:77:ARG:O	2.40	0.42
1:A:232:MET:O	1:A:236:ILE:HG13	2.20	0.41
1:C:172:ASN:O	1:C:288:ARG:HG2	2.20	0.41
1:A:49:PRO:HB3	1:A:70:VAL:HG22	2.03	0.41
1:B:186:THR:O	1:B:190:LYS:HG2	2.21	0.41
1:C:325:PHE:HE1	1:C:358:ILE:HG21	1.84	0.41
1:F:309:LEU:HA	1:F:309:LEU:HD23	1.93	0.41
1:C:149:VAL:O	1:C:153:VAL:HG23	2.21	0.41
1:B:102:LYS:HB3	1:B:102:LYS:HE2	1.79	0.41
1:D:29:ARG:NH2	1:D:61:SER:OG	2.54	0.41
1:F:365:ARG:HB3	1:F:369:THR:OG1	2.20	0.41
1:B:367:GLU:O	1:B:371:ILE:N	2.41	0.41
1:C:63:ASN:HA	1:C:66:PHE:CE1	2.55	0.41
1:C:90:ILE:HG23	1:C:95:ILE:HD13	2.03	0.41
1:A:162:LYS:HB3	1:F:341:ILE:HB	2.03	0.41
1:A:341:ILE:HG23	1:B:162:LYS:HB3	2.03	0.41
1:C:362:LYS:HD3	1:C:362:LYS:HA	1.89	0.41
1:D:281:LEU:HB3	1:D:312:ARG:NH1	2.25	0.41
1:B:219:SER:HA	1:B:257:LEU:HD23	2.03	0.41
1:C:214:SER:HA	1:C:215:HIS:HA	1.64	0.41
1:A:214:SER:HA	1:A:215:HIS:HA	1.55	0.41
1:B:254:VAL:HG23	1:B:298:THR:O	2.21	0.41
1:D:248:PHE:HE1	1:D:294:LEU:HD23	1.86	0.41
1:F:237:ASP:OD1	1:F:290:ARG:NE	2.53	0.41
1:D:232:MET:O	1:D:236:ILE:HG13	2.21	0.40
1:F:180:PRO:HA	1:F:181:PRO:HD3	1.93	0.40
1:B:173:ARG:N	1:B:314:ASP:OD2	2.54	0.40
1:D:8:LEU:HD23	1:D:88:LEU:HD22	2.02	0.40
1:E:233:PHE:HD1	1:E:287:ILE:HD11	1.85	0.40
1:F:363:ALA:HA	1:F:364:PRO:HD3	1.99	0.40
1:F:104:GLY:N	1:F:105:PRO:HD3	2.36	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	366/424 (86%)	358 (98%)	8 (2%)	0	100	100
1	B	374/424 (88%)	366 (98%)	8 (2%)	0	100	100
1	C	364/424 (86%)	354 (97%)	9 (2%)	1 (0%)	46	57
1	D	369/424 (87%)	362 (98%)	7 (2%)	0	100	100
1	E	371/424 (88%)	363 (98%)	8 (2%)	0	100	100
1	F	368/424 (87%)	358 (97%)	10 (3%)	0	100	100
All	All	2212/2544 (87%)	2161 (98%)	50 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	303	SER

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	339/386 (88%)	328 (97%)	11 (3%)	46	62
1	B	343/386 (89%)	328 (96%)	15 (4%)	35	46
1	C	329/386 (85%)	318 (97%)	11 (3%)	45	61
1	D	338/386 (88%)	330 (98%)	8 (2%)	57	74
1	E	336/386 (87%)	320 (95%)	16 (5%)	31	42
1	F	329/386 (85%)	314 (95%)	15 (5%)	33	44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2014/2316 (87%)	1938 (96%)	76 (4%)	40 54

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	32	GLU
1	A	62	LEU
1	A	89	THR
1	A	96	HIS
1	A	126	GLN
1	A	137	GLU
1	A	230	GLN
1	A	252	ASP
1	A	306	ASP
1	A	395	TYR
1	B	18	CYS
1	B	35	GLU
1	B	100	LEU
1	B	102	LYS
1	B	103	ASP
1	B	137	GLU
1	B	173	ARG
1	B	215	HIS
1	B	227	LYS
1	B	228	LEU
1	B	277	VAL
1	B	305	LEU
1	B	353	TYR
1	B	368	PHE
1	B	395	TYR
1	C	43	ASN
1	C	55	LEU
1	C	56	PHE
1	C	89	THR
1	C	175	ILE
1	C	237	ASP
1	C	288	ARG
1	C	347	ASN
1	C	369	THR
1	C	395	TYR
1	C	401	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	86	ASN
1	D	89	THR
1	D	188	LEU
1	D	231	LYS
1	D	232	MET
1	D	255	GLU
1	D	361	THR
1	D	395	TYR
1	E	10	ASN
1	E	65	LEU
1	E	103	ASP
1	E	124	LEU
1	E	137	GLU
1	E	158	ARG
1	E	215	HIS
1	E	216	SER
1	E	222	PHE
1	E	255	GLU
1	E	278	ASN
1	E	306	ASP
1	E	352	ASP
1	E	395	TYR
1	E	400	GLU
1	E	402	THR
1	F	23	LYS
1	F	24	SER
1	F	55	LEU
1	F	59	ASP
1	F	103	ASP
1	F	133	ASP
1	F	137	GLU
1	F	151	SER
1	F	177	LEU
1	F	214	SER
1	F	306	ASP
1	F	356	GLN
1	F	368	PHE
1	F	395	TYR
1	F	422	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	84	ASN
1	A	91	ASN
1	A	123	GLN
1	A	215	HIS
1	A	278	ASN
1	A	366	ASN
1	B	57	GLN
1	B	94	ASN
1	B	101	HIS
1	B	126	GLN
1	B	138	ASN
1	B	144	ASN
1	B	215	HIS
1	B	235	GLN
1	B	318	ASN
1	B	366	ASN
1	C	63	ASN
1	C	172	ASN
1	C	195	HIS
1	C	278	ASN
1	C	407	ASN
1	D	10	ASN
1	D	123	GLN
1	D	147	ASN
1	D	215	HIS
1	E	170	ASN
1	F	12	HIS
1	F	27	GLN
1	F	94	ASN
1	F	138	ASN
1	F	170	ASN
1	F	283	GLN
1	F	318	ASN
1	F	356	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 ⓘ

9 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	501	-	4,4,4	0.14	0	6,6,6	0.09	0
3	ADP	B	501	-	24,29,29	1.01	1 (4%)	23,45,45	1.73	2 (8%)
2	SO4	C	501	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	D	501	-	4,4,4	0.23	0	6,6,6	0.15	0
2	SO4	D	502	-	4,4,4	0.13	0	6,6,6	0.09	0
2	SO4	E	501	-	4,4,4	0.18	0	6,6,6	0.11	0
2	SO4	E	502	-	4,4,4	0.15	0	6,6,6	0.17	0
3	ADP	E	503	-	24,29,29	0.98	1 (4%)	23,45,45	1.74	2 (8%)
2	SO4	F	501	-	4,4,4	0.22	0	6,6,6	0.09	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	501	-	-	0/0/0/0	0/0/0/0
3	ADP	B	501	-	-	0/12/32/32	0/3/3/3
2	SO4	C	501	-	-	0/0/0/0	0/0/0/0
2	SO4	D	501	-	-	0/0/0/0	0/0/0/0
2	SO4	D	502	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	E	501	-	-	0/0/0/0	0/0/0/0
2	SO4	E	502	-	-	0/0/0/0	0/0/0/0
3	ADP	E	503	-	-	0/12/32/32	0/3/3/3
2	SO4	F	501	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	503	ADP	C5-C4	3.11	1.47	1.40
3	B	501	ADP	C5-C4	3.24	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	ADP	N3-C2-N1	-6.44	123.81	128.87
3	E	503	ADP	N3-C2-N1	-6.34	123.89	128.87
3	E	503	ADP	C2'-C1'-N9	-2.13	107.76	113.47
3	B	501	ADP	C4'-O4'-C1'	2.08	111.85	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 95th 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 ²)	Q<0.9
1	A	376/424 (88%)	1.27	78 (20%) 1 2	61, 95, 158, 197	0
1	B	382/424 (90%)	1.08	82 (21%) 1 2	48, 84, 137, 160	0
1	C	374/424 (88%)	0.81	54 (14%) 3 5	42, 85, 129, 150	0
1	D	377/424 (88%)	0.50	29 (7%) 16 23	37, 64, 111, 147	0
1	E	379/424 (89%)	0.92	64 (16%) 2 3	38, 77, 140, 166	0
1	F	376/424 (88%)	1.00	54 (14%) 3 5	39, 80, 133, 203	0
All	All	2264/2544 (88%)	0.93	361 (15%) 3 4	37, 83, 139, 203	0

All (361) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	PHE	13.9
1	F	221	TRP	13.0
1	A	221	TRP	12.0
1	F	223	SER	11.6
1	A	220	LYS	10.1
1	F	222	PHE	10.0
1	F	214	SER	8.6
1	B	222	PHE	8.2
1	F	217	LEU	8.1
1	C	275	ARG	8.1
1	B	221	TRP	8.0
1	D	224	GLU	7.9
1	A	305	LEU	7.9
1	C	218	PHE	7.6
1	C	274	ILE	7.5
1	F	225	SER	7.5
1	B	218	PHE	7.4
1	B	358	ILE	7.4
1	A	26	VAL	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	363	ALA	7.2
1	A	92	PRO	7.2
1	F	220	LYS	7.1
1	E	51	SER	6.9
1	B	107	SER	6.9
1	B	303	SER	6.9
1	F	215	HIS	6.8
1	A	304	THR	6.8
1	B	362	LYS	6.6
1	F	104	GLY	6.6
1	E	65	LEU	6.6
1	B	223	SER	6.5
1	E	222	PHE	6.5
1	A	308	ALA	6.3
1	F	216	SER	6.2
1	E	20	LYS	6.0
1	E	225	SER	6.0
1	A	27	GLN	6.0
1	F	226	GLY	6.0
1	E	221	TRP	5.9
1	B	348	GLU	5.8
1	E	223	SER	5.8
1	A	29	ARG	5.8
1	F	102	LYS	5.7
1	C	222	PHE	5.6
1	B	231	LYS	5.6
1	A	25	THR	5.5
1	E	85	VAL	5.5
1	A	28	LYS	5.4
1	B	364	PRO	5.4
1	F	306	ASP	5.4
1	E	64	GLU	5.3
1	A	215	HIS	5.2
1	D	223	SER	5.2
1	A	280	LEU	5.2
1	F	84	ASN	5.1
1	B	349	VAL	5.1
1	B	276	ALA	5.0
1	E	25	THR	5.0
1	A	303	SER	5.0
1	A	7	THR	5.0
1	E	63	ASN	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	224	GLU	5.0
1	D	89	THR	4.9
1	C	104	GLY	4.9
1	A	225	SER	4.9
1	A	102	LYS	4.9
1	B	354	TRP	4.8
1	A	217	LEU	4.8
1	C	220	LYS	4.8
1	E	86	ASN	4.8
1	E	88	LEU	4.7
1	F	350	HIS	4.7
1	C	276	ALA	4.7
1	A	276	ALA	4.6
1	A	424	ASN	4.6
1	C	219	SER	4.5
1	F	274	ILE	4.5
1	E	21	PHE	4.4
1	E	304	THR	4.4
1	B	20	LYS	4.4
1	B	228	LEU	4.4
1	B	220	LYS	4.4
1	B	359	CYS	4.4
1	E	36	LEU	4.3
1	B	108	GLN	4.3
1	B	353	TYR	4.3
1	A	214	SER	4.2
1	F	278	ASN	4.2
1	B	274	ILE	4.2
1	F	276	ALA	4.2
1	E	305	LEU	4.1
1	F	219	SER	4.1
1	E	37	ILE	4.1
1	A	107	SER	4.1
1	E	303	SER	4.1
1	F	27	GLN	4.0
1	C	92	PRO	4.0
1	A	100	LEU	3.9
1	B	21	PHE	3.9
1	A	307	LYS	3.9
1	D	87	ASP	3.9
1	E	360	ASP	3.9
1	A	226	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	224	GLU	3.8
1	A	61	SER	3.8
1	A	104	GLY	3.7
1	A	309	LEU	3.7
1	A	231	LYS	3.7
1	A	22	PRO	3.7
1	A	301	LEU	3.7
1	A	321	GLN	3.7
1	E	28	LYS	3.7
1	A	238	GLU	3.6
1	C	304	THR	3.6
1	A	30	PHE	3.5
1	A	5	MET	3.5
1	C	214	SER	3.5
1	C	217	LEU	3.5
1	E	26	VAL	3.5
1	C	102	LYS	3.4
1	E	220	LYS	3.4
1	C	103	ASP	3.4
1	C	56	PHE	3.4
1	A	224	GLU	3.4
1	C	166	THR	3.4
1	F	22	PRO	3.4
1	D	51	SER	3.4
1	E	235	GLN	3.4
1	B	350	HIS	3.4
1	C	93	SER	3.4
1	C	278	ASN	3.3
1	A	223	SER	3.3
1	F	275	ARG	3.3
1	B	420	LEU	3.3
1	E	66	PHE	3.3
1	A	422	ARG	3.3
1	A	91	ASN	3.3
1	B	305	LEU	3.3
1	B	301	LEU	3.3
1	C	229	VAL	3.3
1	C	221	TRP	3.3
1	C	76	LEU	3.2
1	B	9	LYS	3.2
1	C	399	PRO	3.2
1	B	295	ILE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	219	SER	3.2
1	B	8	LEU	3.2
1	F	155	ALA	3.1
1	E	218	PHE	3.1
1	F	171	VAL	3.1
1	C	107	SER	3.1
1	E	50	ILE	3.1
1	A	21	PHE	3.1
1	B	360	ASP	3.0
1	F	229	VAL	3.0
1	D	61	SER	3.0
1	A	320	GLY	3.0
1	E	22	PRO	3.0
1	C	108	GLN	3.0
1	E	90	ILE	3.0
1	A	306	ASP	3.0
1	F	153	VAL	3.0
1	E	9	LYS	3.0
1	D	103	ASP	2.9
1	E	302	GLU	2.9
1	A	88	LEU	2.9
1	A	31	SER	2.9
1	B	352	ASP	2.9
1	D	85	VAL	2.9
1	E	362	LYS	2.9
1	A	278	ASN	2.9
1	D	86	ASN	2.9
1	B	230	GLN	2.9
1	B	132	PHE	2.9
1	A	106	LEU	2.9
1	A	17	ILE	2.9
1	A	23	LYS	2.9
1	B	227	LYS	2.9
1	F	218	PHE	2.9
1	A	277	VAL	2.9
1	C	81	LEU	2.9
1	B	202	ASP	2.9
1	C	287	ILE	2.9
1	A	382	LEU	2.9
1	F	228	LEU	2.9
1	E	287	ILE	2.8
1	C	82	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	277	VAL	2.8
1	B	250	LEU	2.8
1	F	58	GLY	2.8
1	C	289	ARG	2.8
1	F	308	ALA	2.8
1	B	421	SER	2.8
1	C	226	GLY	2.8
1	E	301	LEU	2.8
1	E	83	GLU	2.8
1	C	75	GLU	2.8
1	D	88	LEU	2.7
1	B	225	SER	2.7
1	B	133	ASP	2.7
1	B	234	ASP	2.7
1	A	99	LYS	2.7
1	F	20	LYS	2.7
1	A	90	ILE	2.7
1	A	135	ILE	2.7
1	A	8	LEU	2.7
1	A	35	GLU	2.7
1	A	350	HIS	2.7
1	D	9	LYS	2.7
1	F	302	GLU	2.7
1	E	84	ASN	2.7
1	A	62	LEU	2.7
1	B	217	LEU	2.7
1	C	228	LEU	2.7
1	E	361	THR	2.7
1	B	193	ALA	2.6
1	F	81	LEU	2.6
1	A	216	SER	2.6
1	B	323	SER	2.6
1	F	213	ASN	2.6
1	B	184	GLY	2.6
1	B	296	LEU	2.6
1	C	90	ILE	2.6
1	A	122	SER	2.6
1	B	100	LEU	2.6
1	B	196	LEU	2.6
1	C	288	ARG	2.6
1	A	375	ILE	2.6
1	F	168	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	89	THR	2.6
1	E	33	PHE	2.6
1	F	176	LEU	2.6
1	C	295	ILE	2.6
1	A	275	ARG	2.6
1	A	228	LEU	2.6
1	D	30	PHE	2.6
1	A	242	ASP	2.6
1	C	160	SER	2.5
1	B	235	GLN	2.5
1	C	227	LYS	2.5
1	D	84	ASN	2.5
1	B	175	ILE	2.5
1	E	92	PRO	2.5
1	D	228	LEU	2.5
1	D	83	GLU	2.5
1	D	354	TRP	2.5
1	E	95	ILE	2.5
1	A	205	SER	2.5
1	E	87	ASP	2.5
1	B	258	GLY	2.5
1	D	274	ILE	2.5
1	B	382	LEU	2.5
1	B	10	ASN	2.4
1	B	190	LYS	2.4
1	C	10	ASN	2.4
1	D	8	LEU	2.4
1	B	347	ASN	2.4
1	F	166	THR	2.4
1	B	135	ILE	2.4
1	E	8	LEU	2.4
1	B	325	PHE	2.4
1	A	230	GLN	2.4
1	A	243	GLU	2.4
1	D	60	SER	2.4
1	E	143	SER	2.4
1	B	192	LEU	2.4
1	E	228	LEU	2.4
1	A	139	LEU	2.4
1	A	423	ASN	2.4
1	C	105	PRO	2.3
1	E	34	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	192	LEU	2.3
1	C	27	GLN	2.3
1	D	19	GLN	2.3
1	E	306	ASP	2.3
1	B	189	CYS	2.3
1	A	287	ILE	2.3
1	B	106	LEU	2.3
1	B	188	LEU	2.3
1	E	188	LEU	2.3
1	F	172	ASN	2.3
1	B	22	PRO	2.3
1	C	43	ASN	2.3
1	C	306	ASP	2.3
1	B	19	GLN	2.3
1	E	19	GLN	2.3
1	E	184	GLY	2.3
1	B	23	LYS	2.3
1	B	153	VAL	2.3
1	B	219	SER	2.3
1	C	18	CYS	2.3
1	C	380	ARG	2.3
1	B	368	PHE	2.3
1	B	25	THR	2.2
1	D	275	ARG	2.2
1	B	416	VAL	2.2
1	E	124	LEU	2.2
1	F	159	LEU	2.2
1	C	170	ASN	2.2
1	A	371	ILE	2.2
1	B	351	THR	2.2
1	B	210	LEU	2.2
1	C	422	ARG	2.2
1	A	132	PHE	2.2
1	D	175	ILE	2.2
1	F	235	GLN	2.2
1	B	374	LYS	2.2
1	C	277	VAL	2.2
1	D	214	SER	2.2
1	C	172	ASN	2.2
1	D	189	CYS	2.2
1	B	11	ILE	2.2
1	F	174	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	186	THR	2.2
1	F	199	ARG	2.2
1	F	280	LEU	2.2
1	B	134	SER	2.2
1	C	213	ASN	2.1
1	F	158	ARG	2.1
1	D	31	SER	2.1
1	E	27	GLN	2.1
1	E	422	ARG	2.1
1	B	255	GLU	2.1
1	C	353	TYR	2.1
1	A	373	PHE	2.1
1	E	315	ILE	2.1
1	E	41	SER	2.1
1	F	347	ASN	2.1
1	B	226	GLY	2.1
1	B	302	GLU	2.1
1	C	58	GLY	2.1
1	C	106	LEU	2.1
1	B	215	HIS	2.1
1	E	231	LYS	2.1
1	F	123	GLN	2.1
1	B	186	THR	2.1
1	B	254	VAL	2.1
1	F	149	VAL	2.1
1	E	380	ARG	2.1
1	C	55	LEU	2.1
1	D	296	LEU	2.1
1	F	103	ASP	2.1
1	A	32	GLU	2.1
1	E	226	GLY	2.1
1	C	347	ASN	2.1
1	F	157	ALA	2.1
1	F	97	VAL	2.1
1	B	195	HIS	2.0
1	D	188	LEU	2.0
1	E	106	LEU	2.0
1	E	121	GLY	2.0
1	A	253	GLU	2.0
1	B	224	GLU	2.0
1	F	195	HIS	2.0
1	A	176	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	125	TRP	2.0
1	D	353	TYR	2.0
1	E	32	GLU	2.0
1	A	93	SER	2.0
1	E	103	ASP	2.0
1	C	279	ALA	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, 95th 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(\AA^2)	Q<0.9
2	SO4	D	501	5/5	0.99	0.20	1.33	50,52,66,68	0
2	SO4	A	501	5/5	0.87	0.23	0.24	107,113,114,120	0
3	ADP	E	503	27/27	0.96	0.21	0.09	52,78,91,98	0
3	ADP	B	501	27/27	0.92	0.19	-0.19	63,89,110,115	0
2	SO4	F	501	5/5	0.97	0.14	-0.42	70,73,76,79	0
2	SO4	C	501	5/5	0.98	0.11	-1.56	68,72,73,78	0
2	SO4	E	501	5/5	0.92	0.23	-	103,104,108,111	0
2	SO4	E	502	5/5	0.90	0.19	-	106,108,112,116	0
2	SO4	D	502	5/5	0.91	0.20	-	106,107,109,111	0

6.5 Other polymers [i](#)

There are no such residues in this entry.