



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:48 AM GMT

PDB ID : 3FWC
Title : Sac3:Sus1:Cdc31 complex
Authors : Stewart, M.; Jani, D.
Deposited on : 2009-01-17
Resolution : 2.70 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 (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

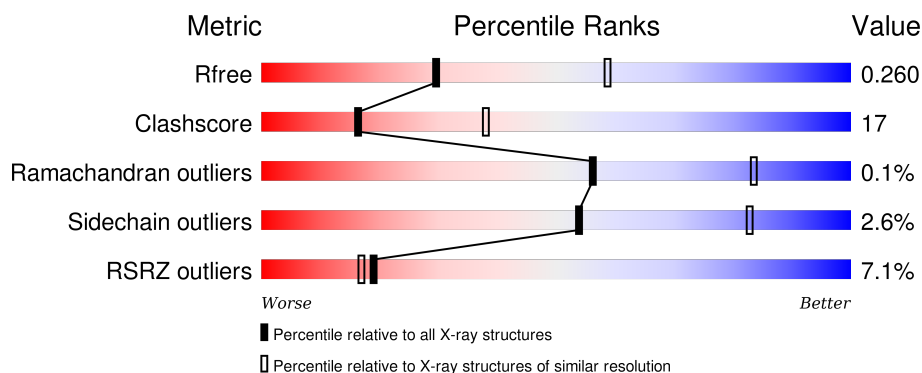
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	161	<div> <div>12%</div> <div> <div>61%</div> <div>29%</div> <div>10%</div> </div> </div>
1	E	161	<div> <div>5%</div> <div> <div>63%</div> <div>26%</div> <div>7%</div> </div> </div>
1	I	161	<div> <div>77%</div> <div>14%</div> <div>9%</div> </div>
1	M	161	<div> <div>2%</div> <div> <div>66%</div> <div>25%</div> <div>8%</div> </div> </div>
2	B	85	<div> <div>6%</div> <div> <div>69%</div> <div>26%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	85	
2	J	85	
2	N	85	
3	C	96	
3	D	96	
3	G	96	
3	H	96	
3	K	96	
3	L	96	
3	O	96	
3	P	96	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13510 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 Cell division control protein 31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	6	0	0
			1197	758	191	242	6			
1	E	150	Total	C	N	O	S	0	0	0
			1233	780	197	250	6			
1	I	147	Total	C	N	O	S	0	0	0
			1213	768	194	245	6			
1	M	148	Total	C	N	O	S	0	0	0
			1221	772	195	248	6			

- Molecule 2 is a protein called Nuclear mRNA export protein SAC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	83	Total	C	N	O	S	0	0	0
			702	449	120	131	2			
2	F	84	Total	C	N	O	S	0	0	0
			708	452	121	133	2			
2	J	78	Total	C	N	O	S	0	0	0
			662	423	113	124	2			
2	N	84	Total	C	N	O	S	0	0	0
			708	452	121	133	2			

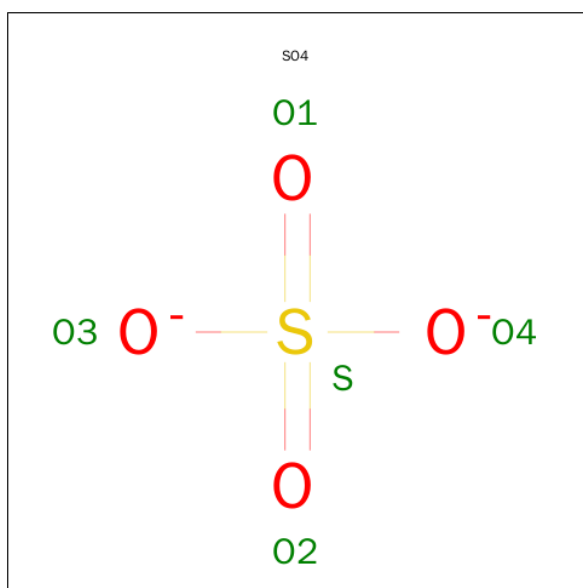
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	721	GLY	-	expression tag	UNP P46674
B	722	SER	-	expression tag	UNP P46674
F	721	GLY	-	expression tag	UNP P46674
F	722	SER	-	expression tag	UNP P46674
J	721	GLY	-	expression tag	UNP P46674
J	722	SER	-	expression tag	UNP P46674
N	721	GLY	-	expression tag	UNP P46674
N	722	SER	-	expression tag	UNP P46674

- Molecule 3 is a protein called Protein SUS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	87	Total	C	N	O	S	13	0	0
			707	444	116	145	2			
3	D	86	Total	C	N	O	S	0	0	0
			697	436	115	144	2			
3	G	88	Total	C	N	O	S	71	0	0
			712	447	117	146	2			
3	H	92	Total	C	N	O	S	0	0	0
			743	464	121	155	3			
3	K	88	Total	C	N	O	S	6	0	0
			712	447	117	146	2			
3	L	84	Total	C	N	O	S	0	0	0
			683	428	112	141	2			
3	O	89	Total	C	N	O	S	38	0	0
			720	451	118	149	2			
3	P	93	Total	C	N	O	S	0	0	0
			750	468	122	157	3			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	M	1	Total	O	S	0	0
			5	4	1		

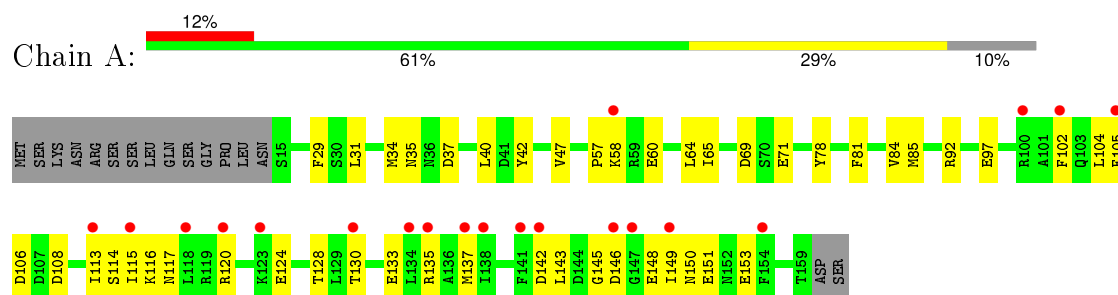
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	C	4	Total	O	0	0
			4	4		
5	D	6	Total	O	0	0
			6	6		
5	E	8	Total	O	0	0
			8	8		
5	F	11	Total	O	0	0
			11	11		
5	G	2	Total	O	0	0
			2	2		
5	H	6	Total	O	0	0
			6	6		
5	I	27	Total	O	0	0
			27	27		
5	J	3	Total	O	0	0
			3	3		
5	K	6	Total	O	0	0
			6	6		
5	L	7	Total	O	0	0
			7	7		
5	M	14	Total	O	0	0
			14	14		
5	N	7	Total	O	0	0
			7	7		
5	O	4	Total	O	0	0
			4	4		
5	P	13	Total	O	0	0
			13	13		

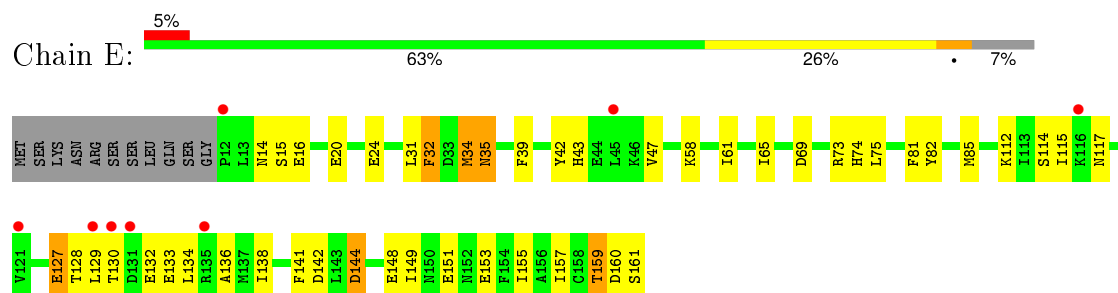
3 Residue-property plots [i](#)

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.

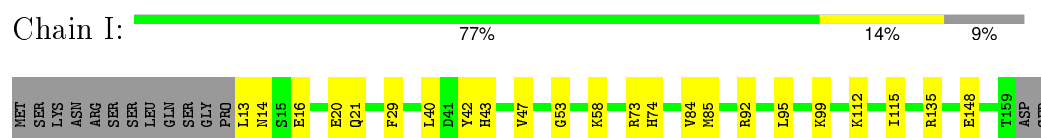
- Molecule 1: Cell division control protein 31



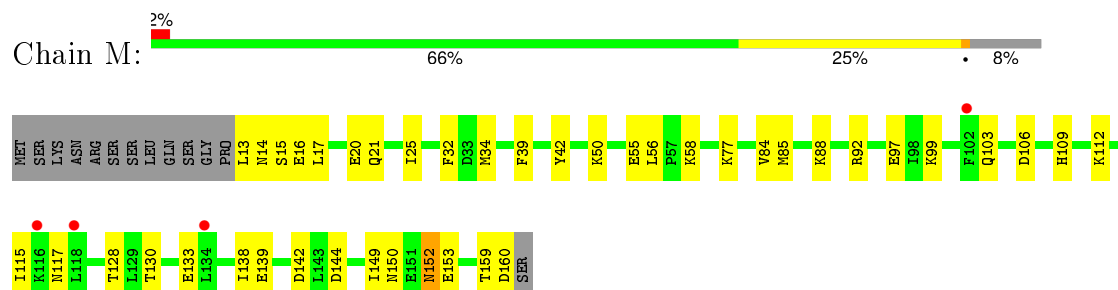
- Molecule 1: Cell division control protein 31



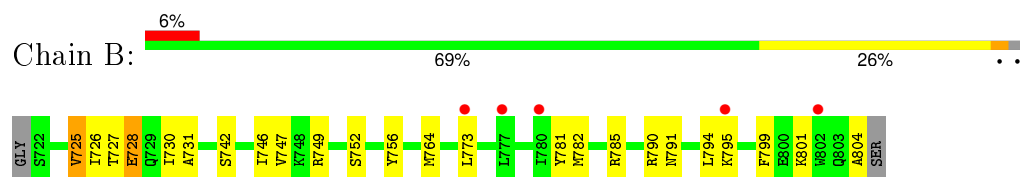
- Molecule 1: Cell division control protein 31



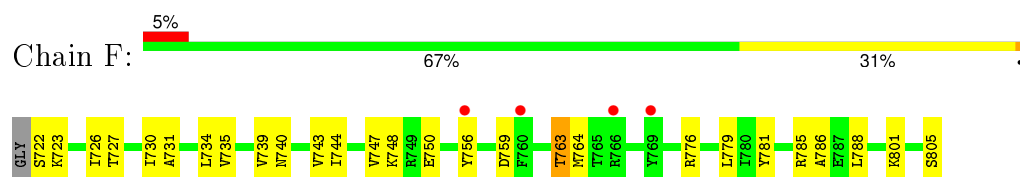
- Molecule 1: Cell division control protein 31



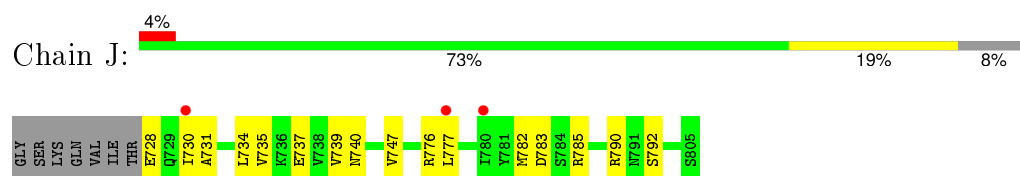
- Molecule 2: Nuclear mRNA export protein SAC3



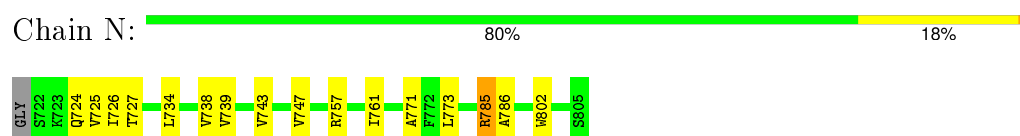
- Molecule 2: Nuclear mRNA export protein SAC3



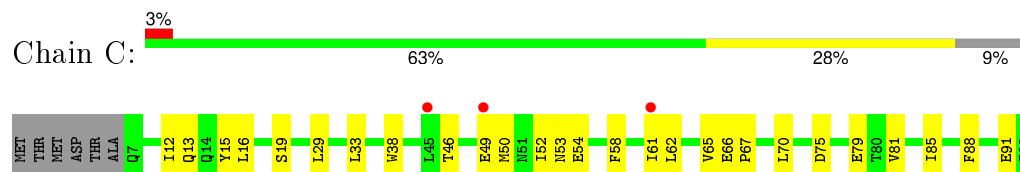
- Molecule 2: Nuclear mRNA export protein SAC3



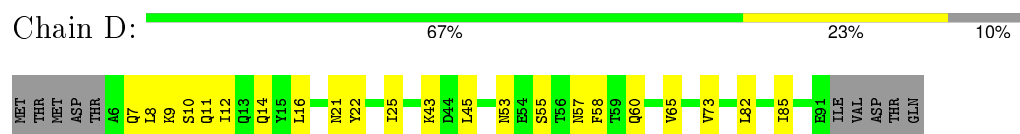
- Molecule 2: Nuclear mRNA export protein SAC3

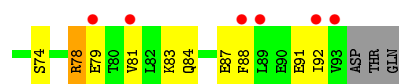


- Molecule 3: Protein SUS1



- Molecule 3: Protein SUS1

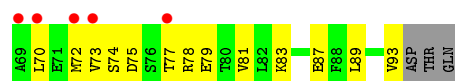
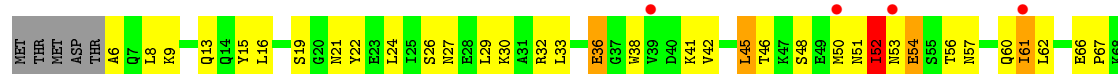
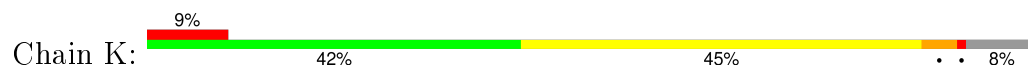




• Molecule 3: Protein SUS1



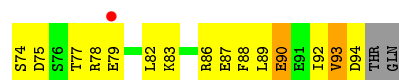
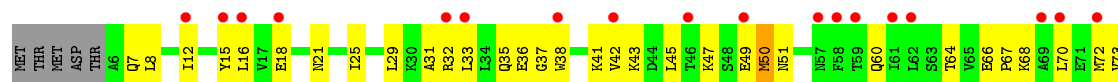
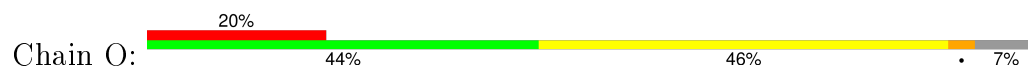
• Molecule 3: Protein SUS1



• Molecule 3: Protein SUS1



• Molecule 3: Protein SUS1



• Molecule 3: Protein SUS1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.59Å 122.71Å 128.71Å 90.00° 95.75° 90.00°	Depositor
Resolution (Å)	19.92 – 2.70 62.88 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.92-2.70) 98.8 (62.88-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.211 , 0.265 0.207 , 0.260	Depositor DCC
R_{free} test set	3094 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 81.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 69154 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13510	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.58 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.3352e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.30	0/1215	0.44	0/1628
1	E	0.33	0/1252	0.44	0/1679
1	I	0.34	0/1231	0.46	0/1650
1	M	0.35	0/1239	0.48	0/1661
2	B	0.32	0/713	0.44	0/955
2	F	0.33	0/719	0.42	0/963
2	J	0.37	0/673	0.44	0/901
2	N	0.43	0/719	0.46	0/963
3	C	0.30	0/713	0.48	0/960
3	D	0.33	0/703	0.45	0/946
3	G	0.31	0/718	0.54	0/967
3	H	0.30	0/749	0.46	0/1009
3	K	0.31	0/718	0.52	0/967
3	L	0.28	0/689	0.43	0/927
3	O	0.29	0/726	0.52	0/978
3	P	0.35	0/756	0.48	0/1019
All	All	0.33	0/13533	0.47	0/18173

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	1197	0	1156	34	0
1	E	1233	0	1187	52	0
1	I	1213	0	1173	15	0
1	M	1221	0	1177	31	0
2	B	702	0	711	31	0
2	F	708	0	716	22	0
2	J	662	0	663	18	0
2	N	708	0	716	19	0
3	C	707	0	718	25	0
3	D	697	0	703	23	0
3	G	712	0	723	51	0
3	H	743	0	747	19	0
3	K	712	0	723	73	0
3	L	683	0	690	20	0
3	O	720	0	727	43	0
3	P	750	0	754	26	0
4	A	5	0	0	0	0
4	G	5	0	0	0	0
4	I	5	0	0	0	0
4	M	5	0	0	0	0
5	A	4	0	0	0	0
5	C	4	0	0	0	0
5	D	6	0	0	0	0
5	E	8	0	0	0	0
5	F	11	0	0	0	0
5	G	2	0	0	0	0
5	H	6	0	0	0	0
5	I	27	0	0	2	0
5	J	3	0	0	0	0
5	K	6	0	0	1	0
5	L	7	0	0	0	0
5	M	14	0	0	0	0
5	N	7	0	0	1	0
5	O	4	0	0	0	0
5	P	13	0	0	1	0
All	All	13510	0	13284	442	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 (442) 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)
3:G:34:LEU:CD1	3:G:39:VAL:HG11	1.88	1.04
3:G:34:LEU:HD13	3:G:39:VAL:HG11	1.45	0.97
2:B:726:ILE:HD11	3:D:9:LYS:HA	1.46	0.95
3:G:38:TRP:CE2	3:G:42:VAL:HG21	2.05	0.91
3:O:32:ARG:HD3	3:O:77:THR:HB	1.51	0.90
3:K:42:VAL:HA	3:K:45:LEU:HD11	1.56	0.86
1:M:159:THR:O	1:M:160:ASP:HB2	1.79	0.81
3:K:51:ASN:HA	3:K:52:ILE:C	2.01	0.81
1:M:42:TYR:OH	1:M:58:LYS:HG2	1.80	0.81
3:O:33:LEU:HD21	3:O:73:VAL:HG23	1.63	0.80
3:K:42:VAL:HA	3:K:45:LEU:CD1	2.11	0.80
3:K:52:ILE:HB	3:K:54:GLU:HB2	1.64	0.79
3:C:50:MET:O	3:C:53:ASN:HB3	1.83	0.78
1:A:42:TYR:OH	1:A:58:LYS:HG2	1.82	0.78
2:B:726:ILE:HD11	3:D:9:LYS:CA	2.14	0.76
3:G:33:LEU:HD13	3:G:38:TRP:CZ3	2.21	0.76
1:I:58:LYS:HE2	5:I:163:HOH:O	1.86	0.74
3:K:52:ILE:HD13	3:K:52:ILE:N	2.03	0.73
3:G:33:LEU:HD13	3:G:38:TRP:CE3	2.24	0.72
3:K:52:ILE:CG1	3:K:54:GLU:HB2	2.21	0.71
1:M:15:SER:HB3	1:M:16:GLU:HA	1.73	0.70
1:A:142:ASP:HB3	1:A:149:ILE:HD13	1.74	0.69
1:A:115:ILE:HD13	1:A:135:ARG:NE	2.06	0.69
1:A:146:ASP:O	1:A:148:GLU:HG2	1.91	0.69
1:A:106:ASP:HB2	1:A:113:ILE:HD13	1.74	0.69
1:E:47:VAL:HG12	2:F:786:ALA:HB2	1.75	0.69
3:G:38:TRP:CE2	3:G:42:VAL:CG2	2.75	0.69
1:E:155:ILE:O	1:E:159:THR:HB	1.93	0.69
3:D:45:LEU:HD23	3:D:65:VAL:HG13	1.76	0.68
1:E:39:PHE:HB3	1:E:75:LEU:HD23	1.76	0.68
3:K:29:LEU:HD13	3:K:81:VAL:HG21	1.76	0.67
3:O:33:LEU:HD22	3:O:38:TRP:CG	2.30	0.66
1:E:130:THR:HB	1:E:133:GLU:HG3	1.78	0.66
3:K:54:GLU:O	3:K:56:THR:HG23	1.95	0.66
3:C:61:ILE:O	3:C:65:VAL:HG22	1.96	0.66
3:K:52:ILE:H	3:K:52:ILE:HD13	1.61	0.66
3:G:39:VAL:HG22	3:G:40:ASP:N	2.10	0.66
2:B:773:LEU:HD12	3:C:29:LEU:HD21	1.78	0.66
3:G:25:ILE:HD12	3:G:84:GLN:HG2	1.77	0.65
3:K:66:GLU:O	3:K:70:LEU:HD12	1.97	0.65
3:O:83:LYS:O	3:O:87:GLU:HB2	1.97	0.65
3:P:8:LEU:O	3:P:12:ILE:HG12	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:29:LEU:O	3:K:33:LEU:HG	1.97	0.65
3:G:78:ARG:O	3:G:81:VAL:HG12	1.97	0.64
1:I:42:TYR:OH	1:I:58:LYS:HG2	1.96	0.64
3:G:78:ARG:HD2	3:G:79:GLU:HG2	1.79	0.64
3:C:29:LEU:HD13	3:C:81:VAL:HG21	1.80	0.63
2:B:726:ILE:HD11	3:D:9:LYS:CB	2.28	0.63
1:A:105:PHE:HB3	1:A:113:ILE:HD12	1.81	0.63
3:O:38:TRP:CE2	3:O:42:VAL:HG21	2.33	0.63
3:L:9:LYS:O	3:L:12:ILE:HG22	1.99	0.63
3:H:46:THR:O	3:H:50:MET:HB2	1.99	0.62
1:M:149:ILE:HG23	1:M:153:GLU:HB2	1.80	0.62
2:J:728:GLU:N	3:L:82:LEU:HD21	2.14	0.62
1:A:114:SER:O	1:A:117:ASN:HB2	2.00	0.62
1:E:130:THR:HG22	1:E:132:GLU:H	1.65	0.62
3:K:48:SER:O	3:K:51:ASN:O	2.17	0.62
3:C:49:GLU:O	3:C:52:ILE:HG22	2.00	0.61
3:K:54:GLU:HG3	3:K:54:GLU:O	2.01	0.61
3:G:34:LEU:HD12	3:G:39:VAL:HG11	1.78	0.61
3:K:79:GLU:HA	3:K:79:GLU:OE1	2.01	0.61
1:E:75:LEU:N	1:E:75:LEU:HD12	2.15	0.61
1:A:102:PHE:CE2	1:A:151:GLU:HB2	2.35	0.61
3:K:52:ILE:CB	3:K:54:GLU:HB2	2.29	0.61
2:B:730:ILE:HG22	3:D:85:ILE:HD13	1.83	0.60
2:F:726:ILE:HD12	3:H:9:LYS:HB2	1.82	0.60
3:K:26:SER:O	3:K:30:LYS:HG3	2.01	0.60
2:F:759:ASP:O	2:F:763:THR:HG23	2.02	0.60
3:G:41:LYS:O	3:G:45:LEU:HD13	2.01	0.60
3:K:62:LEU:O	3:K:66:GLU:HB2	2.02	0.60
3:K:46:THR:O	3:K:50:MET:HG3	2.02	0.59
2:F:734:LEU:HD12	3:H:22:TYR:CE1	2.36	0.59
3:K:46:THR:HG23	3:K:61:ILE:HD11	1.83	0.59
3:D:12:ILE:N	3:D:12:ILE:HD12	2.17	0.59
1:E:74:HIS:C	1:E:75:LEU:HD12	2.23	0.59
2:J:776:ARG:NH2	3:K:30:LYS:HE2	2.18	0.59
1:A:71:GLU:HA	1:A:71:GLU:OE1	2.03	0.59
2:J:734:LEU:HD13	3:L:22:TYR:CZ	2.38	0.59
1:A:133:GLU:O	1:A:137:MET:HG3	2.02	0.59
2:N:785:ARG:HH11	3:O:50:MET:HE1	1.68	0.59
1:I:115:ILE:HD13	1:I:135:ARG:NH2	2.17	0.59
3:K:52:ILE:CG1	3:K:54:GLU:CB	2.81	0.58
3:G:38:TRP:CD2	3:G:42:VAL:HG21	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:66:GLU:HG2	3:K:70:LEU:HD11	1.85	0.58
2:J:739:VAL:HG23	3:L:38:TRP:CZ2	2.38	0.58
3:C:46:THR:O	3:C:50:MET:HG3	2.02	0.58
1:E:132:GLU:HG3	3:O:18:GLU:O	2.03	0.58
3:C:66:GLU:N	3:C:67:PRO:HD2	2.18	0.58
3:G:27:ASN:OD1	3:G:28:GLU:N	2.36	0.58
3:G:39:VAL:CG2	3:G:40:ASP:N	2.64	0.58
3:K:52:ILE:HG12	3:K:54:GLU:CB	2.34	0.58
1:A:65:ILE:O	1:A:69:ASP:HB2	2.03	0.58
3:C:52:ILE:O	3:C:52:ILE:HG23	2.03	0.58
1:E:161:SER:HA	2:F:801:LYS:NZ	2.18	0.58
3:G:83:LYS:O	3:G:87:GLU:HB3	2.03	0.57
1:E:138:ILE:O	1:E:142:ASP:HB2	2.04	0.57
2:N:757:ARG:NE	3:O:94:ASP:O	2.38	0.57
1:E:128:THR:O	1:E:129:LEU:HD23	2.04	0.57
3:G:38:TRP:O	3:G:42:VAL:HG23	2.03	0.57
3:P:95:THR:O	3:P:95:THR:HG22	2.05	0.57
3:O:70:LEU:O	3:O:73:VAL:HG12	2.05	0.57
1:E:42:TYR:OH	1:E:58:LYS:HG2	2.04	0.57
3:G:21:ASN:O	3:G:25:ILE:HG12	2.06	0.56
3:G:36:GLU:HG3	3:G:74:SER:HB2	1.88	0.56
3:L:70:LEU:O	3:L:73:VAL:HG22	2.05	0.56
1:E:151:GLU:O	1:E:155:ILE:HG13	2.04	0.56
1:A:143:LEU:HD12	1:A:143:LEU:O	2.06	0.56
1:A:92:ARG:HD3	1:A:97:GLU:OE2	2.06	0.56
3:O:66:GLU:N	3:O:67:PRO:HD2	2.21	0.55
1:M:106:ASP:OD1	1:M:112:LYS:O	2.24	0.55
2:B:749:ARG:HH21	3:D:43:LYS:CE	2.20	0.55
2:B:799:PHE:C	2:B:799:PHE:CD2	2.79	0.55
3:C:50:MET:O	3:C:53:ASN:CB	2.54	0.55
2:F:730:ILE:HG22	3:H:85:ILE:HD13	1.87	0.55
3:P:66:GLU:HB2	3:P:67:PRO:HD3	1.88	0.55
1:A:57:PRO:HD2	1:A:60:GLU:HG3	1.87	0.55
3:O:93:VAL:HG23	3:O:94:ASP:C	2.27	0.55
2:F:744:ILE:O	2:F:748:LYS:HG2	2.06	0.55
3:K:45:LEU:H	3:K:45:LEU:HD12	1.71	0.55
3:K:70:LEU:O	3:K:73:VAL:HG12	2.06	0.55
1:M:159:THR:O	1:M:160:ASP:CB	2.54	0.54
3:P:70:LEU:HD11	3:P:78:ARG:NH2	2.22	0.54
3:K:36:GLU:OE1	3:K:77:THR:HG21	2.07	0.54
3:L:66:GLU:HB2	3:L:67:PRO:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:87:GLU:O	3:G:91:GLU:OE1	2.25	0.54
1:M:92:ARG:HD3	1:M:97:GLU:CD	2.28	0.54
3:G:38:TRP:CZ2	3:G:42:VAL:HG21	2.42	0.54
1:E:32:PHE:CD1	1:E:32:PHE:N	2.75	0.54
3:L:83:LYS:O	3:L:87:GLU:HG2	2.08	0.54
3:O:75:ASP:O	3:O:79:GLU:HG2	2.08	0.54
3:K:50:MET:O	3:K:52:ILE:O	2.26	0.54
2:N:773:LEU:HD12	3:O:29:LEU:HD21	1.89	0.54
3:K:27:ASN:HA	3:K:30:LYS:HD2	1.90	0.53
3:L:89:LEU:HD12	3:L:90:GLU:N	2.23	0.53
3:C:58:PHE:HA	3:C:61:ILE:HG22	1.90	0.53
1:E:128:THR:HG23	1:E:128:THR:O	2.09	0.53
3:P:53:ASN:HB3	3:P:56:THR:OG1	2.08	0.53
3:G:78:ARG:C	3:G:78:ARG:CD	2.77	0.53
1:M:149:ILE:HD12	2:N:802:TRP:CZ2	2.44	0.53
3:O:78:ARG:O	3:O:82:LEU:HD12	2.09	0.53
3:G:33:LEU:HD22	3:G:38:TRP:CE3	2.44	0.53
3:C:33:LEU:HD13	3:C:38:TRP:CE3	2.44	0.53
3:P:12:ILE:HG21	3:P:89:LEU:HD11	1.91	0.52
3:K:8:LEU:HD12	3:K:8:LEU:O	2.09	0.52
2:N:747:VAL:HG12	3:P:58:PHE:CE1	2.45	0.52
1:E:132:GLU:HB2	3:O:18:GLU:OE1	2.09	0.52
1:M:150:ASN:OD1	1:M:153:GLU:HG3	2.09	0.52
1:A:128:THR:O	1:A:128:THR:HG23	2.10	0.52
3:G:27:ASN:HA	3:G:30:LYS:HE3	1.91	0.52
1:A:120:ARG:O	1:A:124:GLU:HB2	2.10	0.52
3:K:32:ARG:HE	3:K:77:THR:HG22	1.74	0.52
1:E:15:SER:HB2	1:E:16:GLU:OE1	2.10	0.52
2:B:801:LYS:O	2:B:804:ALA:HB3	2.10	0.52
3:O:49:GLU:OE1	3:O:64:THR:HG21	2.09	0.52
3:C:50:MET:O	3:C:53:ASN:N	2.43	0.52
1:E:14:ASN:HB3	1:E:82:TYR:HE2	1.75	0.52
3:K:29:LEU:HG	3:K:33:LEU:HD11	1.92	0.51
2:N:738:VAL:HG21	3:P:29:LEU:HD23	1.92	0.51
3:O:7:GLN:HG3	3:O:8:LEU:H	1.74	0.51
1:E:149:ILE:HG23	1:E:153:GLU:HB2	1.92	0.51
3:C:58:PHE:CZ	3:C:62:LEU:HD12	2.46	0.51
2:F:740:ASN:O	2:F:744:ILE:HG13	2.11	0.51
1:I:13:LEU:HB3	1:I:14:ASN:CB	2.41	0.51
2:B:747:VAL:HG12	3:D:58:PHE:CE1	2.46	0.51
3:D:11:GLN:O	3:D:14:GLN:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:88:PHE:O	3:O:92:ILE:HD12	2.10	0.51
1:A:47:VAL:HG11	2:B:782:MET:HB3	1.93	0.50
2:B:725:VAL:HG22	2:B:728:GLU:CD	2.32	0.50
3:O:74:SER:HG	3:O:77:THR:HG23	1.76	0.50
3:L:16:LEU:HD11	3:L:85:ILE:HG13	1.93	0.50
1:M:115:ILE:HG12	1:M:138:ILE:CD1	2.40	0.50
1:E:75:LEU:N	1:E:75:LEU:CD1	2.74	0.50
3:K:42:VAL:O	3:K:45:LEU:HD12	2.10	0.50
2:N:761:ILE:HD11	3:O:93:VAL:HG21	1.94	0.50
3:L:73:VAL:O	3:L:73:VAL:HG23	2.10	0.50
1:E:114:SER:H	1:E:117:ASN:HB2	1.77	0.50
3:K:32:ARG:NE	3:K:77:THR:HG22	2.27	0.50
2:N:757:ARG:NH2	3:O:90:GLU:HG3	2.26	0.50
3:K:41:LYS:HB3	3:K:72:MET:HE1	1.93	0.50
3:H:12:ILE:HD13	3:H:89:LEU:HD11	1.93	0.50
3:G:33:LEU:HD22	3:G:38:TRP:CD2	2.46	0.50
3:L:86:ARG:HA	3:L:89:LEU:HG	1.94	0.50
1:M:15:SER:HA	1:M:17:LEU:H	1.76	0.50
2:N:734:LEU:HD12	3:P:22:TYR:CE1	2.46	0.50
3:K:15:TYR:O	3:K:19:SER:CB	2.60	0.49
3:G:68:LYS:O	3:G:71:GLU:HG2	2.11	0.49
3:O:88:PHE:O	3:O:92:ILE:CD1	2.60	0.49
3:G:64:THR:O	3:G:68:LYS:HE3	2.12	0.49
2:B:726:ILE:CG2	2:B:727:THR:N	2.75	0.49
3:L:82:LEU:O	3:L:85:ILE:HG22	2.12	0.49
3:D:73:VAL:O	3:D:73:VAL:HG23	2.12	0.49
1:E:31:LEU:HB3	1:E:32:PHE:CD1	2.47	0.49
1:I:29:PHE:CE1	1:I:40:LEU:HG	2.47	0.49
2:B:726:ILE:HG23	2:B:727:THR:N	2.28	0.49
3:G:36:GLU:OE1	3:G:36:GLU:C	2.51	0.49
3:K:38:TRP:O	3:K:42:VAL:HG23	2.12	0.49
1:E:73:ARG:HB3	1:E:75:LEU:HD13	1.93	0.49
2:F:739:VAL:O	2:F:743:VAL:HG23	2.11	0.49
1:E:69:ASP:OD2	1:E:73:ARG:O	2.30	0.49
3:D:58:PHE:HB2	1:I:13:LEU:HD23	1.93	0.49
1:I:13:LEU:HB3	1:I:14:ASN:CA	2.43	0.49
3:P:92:ILE:CG2	3:P:93:VAL:N	2.76	0.49
1:E:34:MET:CE	1:E:34:MET:HA	2.43	0.49
3:K:66:GLU:N	3:K:67:PRO:HD2	2.28	0.49
3:G:78:ARG:C	3:G:78:ARG:HD3	2.32	0.49
3:D:8:LEU:HD13	3:D:11:GLN:NE2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:92:ILE:HG22	3:H:92:ILE:O	2.12	0.49
1:M:21:GLN:O	1:M:25:ILE:HG13	2.13	0.49
2:F:743:VAL:O	2:F:747:VAL:HG23	2.13	0.49
3:K:52:ILE:N	3:K:52:ILE:CD1	2.71	0.48
3:D:7:GLN:OE1	3:D:7:GLN:HA	2.13	0.48
1:I:112:LYS:HD3	1:I:148:GLU:OE1	2.13	0.48
2:B:727:THR:HG22	3:D:82:LEU:HD11	1.94	0.48
3:K:52:ILE:H	3:K:52:ILE:CD1	2.25	0.48
1:E:130:THR:HG21	3:O:18:GLU:OE1	2.13	0.48
1:E:138:ILE:HA	1:E:149:ILE:HD11	1.95	0.48
1:E:32:PHE:CE2	1:E:47:VAL:CG1	2.96	0.48
3:H:16:LEU:HD13	3:H:88:PHE:CD2	2.49	0.48
3:O:74:SER:OG	3:O:77:THR:HG23	2.13	0.48
1:A:106:ASP:HB2	1:A:113:ILE:CD1	2.43	0.48
1:A:34:MET:HE3	2:B:782:MET:SD	2.53	0.48
3:G:34:LEU:HD12	3:G:39:VAL:CG1	2.44	0.48
3:O:43:LYS:O	3:O:47:LYS:HB2	2.13	0.48
3:P:11:GLN:O	3:P:15:TYR:HD1	1.97	0.48
1:A:106:ASP:OD1	1:A:108:ASP:OD1	2.32	0.48
1:M:152:ASN:N	1:M:152:ASN:OD1	2.46	0.48
3:G:29:LEU:O	3:G:33:LEU:HD12	2.14	0.47
3:H:25:ILE:O	3:H:28:GLU:HB2	2.14	0.47
2:B:791:ASN:HB3	2:B:795:LYS:HE3	1.96	0.47
1:M:84:VAL:HG12	1:M:85:MET:HE2	1.95	0.47
1:E:141:PHE:HZ	2:F:805:SER:CB	2.28	0.47
3:K:15:TYR:O	3:K:19:SER:HB2	2.14	0.47
2:J:734:LEU:HA	2:J:737:GLU:OE1	2.14	0.47
3:K:16:LEU:HG	3:K:22:TYR:HB2	1.96	0.47
3:P:53:ASN:CB	3:P:56:THR:OG1	2.63	0.47
1:M:39:PHE:CE2	1:M:77:LYS:HB3	2.50	0.47
2:N:739:VAL:O	2:N:743:VAL:HG23	2.14	0.47
3:K:52:ILE:O	3:K:54:GLU:HB3	2.14	0.47
1:E:129:LEU:HD22	1:E:133:GLU:CD	2.35	0.47
2:N:757:ARG:HH21	3:O:90:GLU:HG3	1.78	0.47
2:B:781:TYR:OH	2:B:785:ARG:NH1	2.47	0.47
1:I:20:GLU:HG3	1:I:21:GLN:N	2.28	0.47
1:M:14:ASN:HB3	1:M:15:SER:O	2.14	0.47
3:K:66:GLU:HB3	3:K:67:PRO:CD	2.43	0.47
3:K:41:LYS:CB	3:K:72:MET:HE1	2.44	0.47
3:P:34:LEU:HD13	3:P:39:VAL:HG21	1.96	0.47
3:O:41:LYS:O	3:O:45:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:722:SER:O	2:F:726:ILE:HG12	2.15	0.46
1:E:31:LEU:HD23	1:E:32:PHE:HE1	1.79	0.46
1:E:39:PHE:CB	1:E:75:LEU:HD23	2.43	0.46
2:B:781:TYR:CD2	2:B:782:MET:HE2	2.50	0.46
3:K:89:LEU:O	3:K:93:VAL:HG23	2.16	0.46
3:H:61:ILE:O	3:H:65:VAL:HG23	2.15	0.46
1:E:144:ASP:HB2	1:E:153:GLU:OE2	2.15	0.46
1:I:73:ARG:O	1:I:74:HIS:HB2	2.15	0.46
3:K:52:ILE:HG12	3:K:54:GLU:HB3	1.96	0.46
2:J:730:ILE:HB	3:L:85:ILE:CD1	2.46	0.46
1:E:115:ILE:HD11	1:E:134:LEU:HB2	1.96	0.46
1:A:64:LEU:HD13	1:A:84:VAL:HG11	1.97	0.46
3:G:12:ILE:HD11	3:G:92:ILE:HG21	1.97	0.46
3:K:9:LYS:O	3:K:13:GLN:HG2	2.16	0.46
1:E:159:THR:HG22	1:E:160:ASP:N	2.31	0.46
3:G:84:GLN:HA	3:G:87:GLU:HG2	1.96	0.46
3:O:21:ASN:O	3:O:25:ILE:HG12	2.16	0.46
3:P:68:LYS:O	3:P:72:MET:HG3	2.16	0.46
1:E:133:GLU:O	1:E:136:ALA:HB3	2.16	0.46
3:H:13:GLN:O	3:H:17:VAL:HG23	2.16	0.46
3:K:75:ASP:O	3:K:79:GLU:HG2	2.15	0.46
2:J:735:VAL:O	2:J:739:VAL:HG12	2.16	0.46
2:F:731:ALA:O	2:F:735:VAL:HG23	2.15	0.46
2:J:776:ARG:NH2	3:K:30:LYS:HG2	2.31	0.45
1:M:138:ILE:O	1:M:142:ASP:HB2	2.16	0.45
3:K:83:LYS:O	3:K:87:GLU:HG3	2.16	0.45
2:F:781:TYR:CE2	3:G:62:LEU:HB2	2.51	0.45
2:F:776:ARG:HH12	2:F:779:LEU:HD12	1.81	0.45
3:O:33:LEU:HB3	3:O:38:TRP:CE3	2.51	0.45
2:J:730:ILE:HD11	3:L:13:GLN:HB2	1.97	0.45
1:E:34:MET:HA	1:E:34:MET:HE2	1.98	0.45
1:A:31:LEU:HD11	2:B:785:ARG:HE	1.82	0.45
3:K:51:ASN:CA	3:K:52:ILE:C	2.76	0.45
1:M:92:ARG:HD3	1:M:97:GLU:CG	2.46	0.45
2:J:747:VAL:HG12	3:L:58:PHE:CE1	2.52	0.45
1:A:130:THR:H	1:A:133:GLU:HG3	1.81	0.45
3:P:52:ILE:HG13	3:P:53:ASN:H	1.81	0.45
3:K:32:ARG:NH2	3:K:77:THR:HG22	2.32	0.45
1:M:106:ASP:OD2	1:M:109:HIS:CA	2.65	0.45
3:G:12:ILE:HA	3:G:15:TYR:HB3	1.99	0.45
3:K:45:LEU:HD12	3:K:45:LEU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:130:THR:OG1	1:M:133:GLU:HG3	2.17	0.45
1:M:144:ASP:HB2	1:M:153:GLU:OE2	2.17	0.45
3:P:39:VAL:HG12	3:P:43:LYS:HE2	1.99	0.45
2:B:764:MET:HE3	3:C:12:ILE:HG21	1.99	0.45
2:B:725:VAL:HG22	2:B:728:GLU:OE2	2.17	0.44
1:M:56:LEU:HD11	1:M:88:LYS:HE2	1.98	0.44
3:G:66:GLU:N	3:G:67:PRO:HD3	2.31	0.44
1:M:128:THR:O	1:M:128:THR:HG22	2.17	0.44
3:O:15:TYR:CD2	3:O:15:TYR:C	2.90	0.44
3:K:53:ASN:O	3:K:54:GLU:C	2.55	0.44
1:A:145:GLY:HA2	1:A:146:ASP:HA	1.66	0.44
2:J:782:MET:HA	2:J:782:MET:HE2	1.97	0.44
2:B:790:ARG:NH1	2:B:794:LEU:HD11	2.32	0.44
3:C:66:GLU:O	3:C:70:LEU:HG	2.16	0.44
3:O:8:LEU:O	3:O:12:ILE:HG12	2.17	0.44
3:K:6:ALA:C	3:K:8:LEU:N	2.69	0.44
3:P:64:THR:O	3:P:68:LYS:HD2	2.18	0.44
3:G:36:GLU:OE1	3:G:38:TRP:N	2.51	0.44
1:M:106:ASP:OD2	1:M:109:HIS:N	2.49	0.44
1:E:112:LYS:HD2	1:E:148:GLU:OE1	2.17	0.44
2:B:782:MET:CE	2:B:782:MET:HA	2.48	0.44
3:G:66:GLU:N	3:G:67:PRO:CD	2.81	0.44
1:A:35:ASN:HB2	1:E:35:ASN:O	2.18	0.44
3:H:63:SER:O	3:H:67:PRO:HD2	2.18	0.44
1:M:15:SER:HA	1:M:17:LEU:N	2.33	0.44
3:C:12:ILE:O	3:C:13:GLN:C	2.55	0.44
3:P:56:THR:CG2	3:P:60:GLN:HB2	2.48	0.44
1:A:104:LEU:HD21	2:B:791:ASN:ND2	2.32	0.44
1:E:32:PHE:N	1:E:32:PHE:HD1	2.16	0.44
1:E:81:PHE:CZ	1:E:85:MET:HG3	2.52	0.44
3:K:21:ASN:HA	3:K:24:LEU:HB2	1.99	0.44
2:N:771:ALA:HA	5:N:18:HOH:O	2.17	0.44
2:B:752:SER:O	2:B:756:TYR:CD2	2.71	0.44
1:I:84:VAL:HG12	1:I:85:MET:HE2	1.99	0.44
3:P:52:ILE:HG13	3:P:53:ASN:N	2.33	0.43
2:N:724:GLN:OE1	2:N:724:GLN:HA	2.18	0.43
3:G:34:LEU:HA	3:G:34:LEU:HD12	1.75	0.43
1:M:50:LYS:HE3	1:M:55:GLU:OE2	2.18	0.43
3:O:68:LYS:O	3:O:72:MET:HG3	2.18	0.43
2:J:785:ARG:HH21	3:K:50:MET:HE3	1.84	0.43
3:G:84:GLN:O	3:G:87:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:731:ALA:HA	3:D:85:ILE:HD12	1.99	0.43
2:F:747:VAL:HG12	3:H:58:PHE:CE1	2.54	0.43
3:K:38:TRP:CE2	3:K:42:VAL:HG21	2.54	0.43
3:D:12:ILE:CD1	3:D:12:ILE:N	2.80	0.43
2:B:742:SER:O	2:B:746:ILE:HG13	2.19	0.43
2:B:727:THR:HG22	3:D:82:LEU:CD1	2.49	0.43
3:L:38:TRP:O	3:L:42:VAL:HG23	2.19	0.43
3:K:6:ALA:HA	5:K:100:HOH:O	2.19	0.43
1:A:35:ASN:OD1	1:A:37:ASP:CG	2.57	0.43
3:H:38:TRP:CZ2	3:H:42:VAL:HG21	2.54	0.43
2:F:750:GLU:OE1	3:H:47:LYS:HE3	2.19	0.43
3:C:62:LEU:HD23	3:C:62:LEU:C	2.39	0.43
3:O:35:GLN:C	3:O:37:GLY:H	2.22	0.43
3:K:52:ILE:HG13	3:K:54:GLU:HB2	2.00	0.43
1:I:53:GLY:N	2:J:790:ARG:HD3	2.34	0.43
1:E:20:GLU:O	1:E:24:GLU:HG3	2.19	0.43
3:K:52:ILE:HG13	3:K:54:GLU:CD	2.39	0.42
3:K:54:GLU:CG	3:K:54:GLU:O	2.62	0.42
3:K:32:ARG:HH21	3:K:77:THR:HG22	1.83	0.42
3:O:89:LEU:O	3:O:93:VAL:HG22	2.19	0.42
3:P:92:ILE:HG22	3:P:93:VAL:N	2.34	0.42
2:F:750:GLU:HA	2:F:750:GLU:OE2	2.19	0.42
3:G:46:THR:HG23	3:G:65:VAL:HG11	2.01	0.42
3:D:21:ASN:O	3:D:25:ILE:HG13	2.19	0.42
3:K:29:LEU:O	3:K:33:LEU:CG	2.66	0.42
3:O:92:ILE:N	3:O:92:ILE:HD12	2.34	0.42
3:H:94:ASP:OD1	3:H:94:ASP:C	2.57	0.42
1:A:81:PHE:CZ	1:A:85:MET:HG3	2.55	0.42
3:C:16:LEU:HA	3:C:88:PHE:CZ	2.55	0.42
3:G:78:ARG:CD	3:G:79:GLU:N	2.83	0.42
2:N:726:ILE:HD12	3:P:9:LYS:HB2	2.02	0.42
3:C:75:ASP:O	3:C:79:GLU:HG2	2.19	0.42
1:E:61:ILE:O	1:E:65:ILE:HG13	2.19	0.42
3:K:79:GLU:OE1	3:K:79:GLU:CA	2.67	0.42
3:G:16:LEU:HD13	3:G:88:PHE:CE2	2.54	0.42
2:J:785:ARG:NE	3:K:50:MET:HE1	2.35	0.42
3:K:51:ASN:HA	3:K:53:ASN:N	2.33	0.42
3:C:50:MET:O	3:C:53:ASN:CA	2.68	0.42
1:E:32:PHE:HE2	1:E:47:VAL:CG1	2.33	0.42
2:N:785:ARG:NH1	3:O:50:MET:HE1	2.33	0.42
2:B:749:ARG:HH21	3:D:43:LYS:NZ	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:35:GLN:HB2	5:P:102:HOH:O	2.18	0.42
1:E:127:GLU:OE1	1:E:127:GLU:CA	2.67	0.42
1:M:55:GLU:O	1:M:56:LEU:HD23	2.20	0.42
1:E:31:LEU:HD23	1:E:32:PHE:CE1	2.53	0.42
1:M:149:ILE:HD12	2:N:802:TRP:CH2	2.54	0.42
3:G:26:SER:O	3:G:30:LYS:HG3	2.19	0.42
2:N:727:THR:HG22	3:P:82:LEU:HD12	2.02	0.42
3:P:90:GLU:HA	3:P:90:GLU:OE2	2.20	0.42
3:D:16:LEU:HD23	3:D:22:TYR:HD1	1.84	0.42
3:K:50:MET:HE2	3:K:50:MET:HB3	1.95	0.42
3:C:53:ASN:O	3:C:54:GLU:HB2	2.20	0.42
1:A:116:LYS:HG3	1:A:117:ASN:N	2.34	0.42
3:O:7:GLN:HG3	3:O:8:LEU:N	2.35	0.42
3:O:86:ARG:HB2	3:O:86:ARG:NH1	2.35	0.42
2:J:739:VAL:HG13	2:J:740:ASN:N	2.35	0.41
1:E:141:PHE:CD2	1:E:157:ILE:HG12	2.54	0.41
3:K:57:ASN:H	3:K:60:GLN:HG3	1.84	0.41
2:F:788:LEU:CD1	3:G:47:LYS:HE3	2.50	0.41
2:F:723:LYS:O	2:F:727:THR:HG23	2.21	0.41
1:E:32:PHE:CE2	1:E:47:VAL:HG12	2.55	0.41
2:J:728:GLU:CA	3:L:82:LEU:HD21	2.50	0.41
2:B:781:TYR:HD2	2:B:782:MET:HE2	1.85	0.41
3:C:15:TYR:O	3:C:19:SER:OG	2.35	0.41
3:G:6:ALA:N	3:G:9:LYS:HD2	2.35	0.41
1:E:142:ASP:OD1	1:E:144:ASP:CB	2.68	0.41
3:O:16:LEU:HD12	3:O:21:ASN:HB3	2.01	0.41
1:I:95:LEU:O	1:I:99:LYS:HG3	2.21	0.41
1:A:115:ILE:HD13	1:A:135:ARG:CZ	2.50	0.41
3:G:27:ASN:OD1	3:G:28:GLU:HG3	2.20	0.41
1:E:34:MET:CE	1:E:34:MET:CA	2.99	0.41
2:F:756:TYR:O	2:F:756:TYR:CG	2.73	0.41
1:A:29:PHE:CE1	1:A:40:LEU:HG	2.55	0.41
3:K:29:LEU:HG	3:K:33:LEU:CD1	2.50	0.41
2:F:785:ARG:HA	3:G:50:MET:HE1	2.03	0.41
1:A:142:ASP:HB3	1:A:149:ILE:CD1	2.47	0.41
3:K:74:SER:OG	3:K:77:THR:HG23	2.21	0.41
2:N:727:THR:HG22	3:P:82:LEU:CD1	2.51	0.41
1:M:32:PHE:CZ	2:N:786:ALA:HB2	2.55	0.41
1:A:150:ASN:O	1:A:153:GLU:HB2	2.20	0.41
3:L:26:SER:O	3:L:30:LYS:HG3	2.20	0.41
3:O:36:GLU:OE2	3:O:77:THR:HG21	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:HIS:O	1:E:47:VAL:HG23	2.21	0.41
3:G:71:GLU:OE1	3:G:71:GLU:HA	2.20	0.41
3:K:22:TYR:CD2	3:K:22:TYR:C	2.94	0.41
3:H:66:GLU:HB2	3:H:67:PRO:CD	2.50	0.41
3:G:9:LYS:O	3:G:13:GLN:CB	2.69	0.41
1:A:29:PHE:CG	1:A:78:TYR:HD1	2.39	0.41
3:P:25:ILE:HG23	3:P:84:GLN:OE1	2.21	0.41
3:O:31:ALA:O	3:O:35:GLN:HG3	2.20	0.41
3:C:91:GLU:O	3:C:91:GLU:HG3	2.20	0.41
3:L:29:LEU:O	3:L:33:LEU:HG	2.21	0.41
3:L:43:LYS:O	3:L:47:LYS:HG3	2.20	0.41
1:E:159:THR:CG2	1:E:160:ASP:N	2.80	0.40
3:K:77:THR:O	3:K:81:VAL:HG23	2.21	0.40
3:C:85:ILE:O	3:C:88:PHE:HB3	2.21	0.40
3:D:53:ASN:OD1	3:D:55:SER:N	2.54	0.40
3:D:57:ASN:OD1	3:D:60:GLN:HG3	2.21	0.40
1:I:92:ARG:NH1	5:I:164:HOH:O	2.55	0.40
3:D:9:LYS:HG3	3:D:10:SER:N	2.36	0.40
2:J:731:ALA:O	2:J:735:VAL:HG23	2.22	0.40
1:M:99:LYS:O	1:M:103:GLN:OE1	2.38	0.40
3:H:51:ASN:O	3:H:52:ILE:C	2.60	0.40
3:G:24:LEU:HA	3:G:27:ASN:ND2	2.37	0.40
3:O:92:ILE:HD12	3:O:92:ILE:H	1.86	0.40
2:B:782:MET:HA	2:B:782:MET:HE2	2.03	0.40
3:H:53:ASN:C	3:H:55:SER:H	2.25	0.40
3:O:33:LEU:HD13	3:O:38:TRP:CE3	2.56	0.40
3:H:3:MET:HG3	3:H:7:GLN:HB2	2.02	0.40
2:J:777:LEU:HD12	2:J:777:LEU:HA	1.95	0.40
3:C:33:LEU:HD13	3:C:38:TRP:CZ3	2.57	0.40
1:M:115:ILE:HG12	1:M:138:ILE:HD12	2.02	0.40
1:I:43:HIS:O	1:I:47:VAL:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	143/161 (89%)	138 (96%)	5 (4%)	0	100	100
1	E	148/161 (92%)	139 (94%)	9 (6%)	0	100	100
1	I	145/161 (90%)	142 (98%)	3 (2%)	0	100	100
1	M	146/161 (91%)	143 (98%)	3 (2%)	0	100	100
2	B	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
2	F	82/85 (96%)	81 (99%)	1 (1%)	0	100	100
2	J	76/85 (89%)	74 (97%)	2 (3%)	0	100	100
2	N	82/85 (96%)	81 (99%)	1 (1%)	0	100	100
3	C	85/96 (88%)	77 (91%)	8 (9%)	0	100	100
3	D	84/96 (88%)	80 (95%)	4 (5%)	0	100	100
3	G	86/96 (90%)	80 (93%)	6 (7%)	0	100	100
3	H	90/96 (94%)	85 (94%)	5 (6%)	0	100	100
3	K	86/96 (90%)	74 (86%)	10 (12%)	2 (2%)	8	20
3	L	82/96 (85%)	80 (98%)	2 (2%)	0	100	100
3	O	87/96 (91%)	81 (93%)	6 (7%)	0	100	100
3	P	91/96 (95%)	90 (99%)	1 (1%)	0	100	100
All	All	1594/1752 (91%)	1523 (96%)	69 (4%)	2 (0%)	56	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	52	ILE
3	K	54	GLU

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	130/145 (90%)	130 (100%)	0	100	100
1	E	134/145 (92%)	128 (96%)	6 (4%)	34	65
1	I	132/145 (91%)	131 (99%)	1 (1%)	86	96
1	M	133/145 (92%)	127 (96%)	6 (4%)	34	65
2	B	78/79 (99%)	76 (97%)	2 (3%)	54	83
2	F	79/79 (100%)	77 (98%)	2 (2%)	55	84
2	J	73/79 (92%)	71 (97%)	2 (3%)	52	82
2	N	79/79 (100%)	77 (98%)	2 (2%)	55	84
3	C	83/91 (91%)	83 (100%)	0	100	100
3	D	81/91 (89%)	81 (100%)	0	100	100
3	G	83/91 (91%)	79 (95%)	4 (5%)	31	62
3	H	87/91 (96%)	86 (99%)	1 (1%)	80	94
3	K	83/91 (91%)	78 (94%)	5 (6%)	24	50
3	L	80/91 (88%)	78 (98%)	2 (2%)	55	84
3	O	84/91 (92%)	79 (94%)	5 (6%)	24	50
3	P	88/91 (97%)	87 (99%)	1 (1%)	80	94
All	All	1507/1624 (93%)	1468 (97%)	39 (3%)	54	83

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	725	VAL
2	B	728	GLU
1	E	32	PHE
1	E	34	MET
1	E	35	ASN
1	E	127	GLU
1	E	144	ASP
1	E	159	THR
2	F	763	THR
2	F	764	MET
3	G	36	GLU
3	G	53	ASN
3	G	68	LYS
3	G	78	ARG
3	H	19	SER
1	I	16	GLU

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Mol	Chain	Res	Type
2	J	783	ASP
2	J	792	SER
3	K	36	GLU
3	K	45	LEU
3	K	52	ILE
3	K	61	ILE
3	K	78	ARG
3	L	19	SER
3	L	53	ASN
1	M	13	LEU
1	M	20	GLU
1	M	34	MET
1	M	117	ASN
1	M	139	GLU
1	M	152	ASN
2	N	725	VAL
2	N	785	ARG
3	O	50	MET
3	O	51	ASN
3	O	60	GLN
3	O	90	GLU
3	O	93	VAL
3	P	92	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

4 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	$\# Z > 2$
4	SO4	A	162	-	4,4,4	0.23	0	6,6,6	0.06	0
4	SO4	G	97	-	4,4,4	0.21	0	6,6,6	0.11	0
4	SO4	I	162	-	4,4,4	0.22	0	6,6,6	0.07	0
4	SO4	M	162	-	4,4,4	0.23	0	6,6,6	0.13	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
4	SO4	A	162	-	-	0/0/0/0	0/0/0/0
4	SO4	G	97	-	-	0/0/0/0	0/0/0/0
4	SO4	I	162	-	-	0/0/0/0	0/0/0/0
4	SO4	M	162	-	-	0/0/0/0	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.

No monomer is involved in short contacts.

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, 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	144/161 (89%)	0.75	20 (13%) 4 3	58, 104, 160, 189	0
1	E	150/161 (93%)	0.51	8 (5%) 30 28	52, 92, 145, 175	0
1	I	147/161 (91%)	0.26	0 100 100	42, 70, 110, 136	0
1	M	148/161 (91%)	0.30	4 (2%) 58 58	36, 79, 131, 160	0
2	B	83/85 (97%)	0.60	5 (6%) 25 24	58, 86, 120, 155	0
2	F	84/85 (98%)	0.50	4 (4%) 34 33	59, 91, 121, 140	0
2	J	78/85 (91%)	0.34	3 (3%) 44 44	54, 70, 113, 146	0
2	N	84/85 (98%)	0.34	0 100 100	31, 68, 98, 152	0
3	C	85/96 (88%)	0.33	3 (3%) 48 48	66, 111, 160, 184	0
3	D	86/96 (89%)	0.25	0 100 100	56, 91, 137, 150	0
3	G	80/96 (83%)	1.50	25 (31%) 1 0	94, 150, 204, 220	1 (1%)
3	H	92/96 (95%)	0.36	3 (3%) 50 50	51, 90, 122, 173	0
3	K	87/96 (90%)	0.59	9 (10%) 9 6	61, 116, 157, 172	0
3	L	84/96 (87%)	0.57	6 (7%) 19 17	70, 108, 159, 185	0
3	O	84/96 (87%)	1.15	19 (22%) 1 1	75, 142, 171, 210	0
3	P	93/96 (96%)	0.44	5 (5%) 29 28	37, 69, 145, 165	0
All	All	1609/1752 (91%)	0.53	114 (7%) 19 17	31, 93, 160, 220	1 (0%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	LEU	7.1
3	G	92	ILE	6.9
3	P	95	THR	6.7
3	G	32	ARG	6.0
3	G	93	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	146	ASP	5.5
3	O	15	TYR	5.2
1	E	135	ARG	5.1
3	G	18	GLU	5.1
3	G	16	LEU	5.0
3	O	58	PHE	5.0
3	G	12	ILE	5.0
3	L	32	ARG	4.8
3	G	65	VAL	4.7
3	K	69	ALA	4.6
2	J	730	ILE	4.6
1	A	135	ARG	4.6
3	O	61	ILE	4.5
1	M	134	LEU	4.4
1	E	129	LEU	4.4
3	G	89	LEU	4.3
3	O	70	LEU	4.2
3	O	62	LEU	4.1
3	G	81	VAL	4.0
3	O	49	GLU	3.9
1	E	12	PRO	3.9
3	G	21	ASN	3.8
3	G	79	GLU	3.8
3	K	53	ASN	3.8
1	E	116	LYS	3.7
2	B	802	TRP	3.6
1	A	154	PHE	3.6
3	O	46	THR	3.6
3	O	42	VAL	3.6
3	P	94	ASP	3.6
3	G	88	PHE	3.6
3	G	29	LEU	3.6
1	A	100	ARG	3.5
1	A	105	PHE	3.5
3	K	72	MET	3.5
3	G	15	TYR	3.5
3	G	60	GLN	3.5
3	L	81	VAL	3.4
2	F	756	TYR	3.4
3	K	39	VAL	3.3
1	A	149	ILE	3.3
2	B	773	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	142	ASP	3.3
3	G	38	TRP	3.2
2	F	760	PHE	3.2
3	G	34	LEU	3.2
3	L	92	ILE	3.2
1	A	141	PHE	3.2
3	H	93	VAL	3.2
3	G	50	MET	3.2
3	C	45	LEU	3.1
3	L	25	ILE	3.1
3	G	66	GLU	3.1
3	G	20	GLY	3.1
1	A	113	ILE	3.1
3	G	33	LEU	3.1
3	O	38	TRP	3.1
3	C	49	GLU	3.0
3	H	94	ASP	3.0
3	O	33	LEU	2.9
3	O	79	GLU	2.9
1	A	147	GLY	2.8
3	P	86	ARG	2.8
1	E	130	THR	2.8
1	M	118	LEU	2.7
1	A	138	ILE	2.7
3	O	12	ILE	2.7
3	K	73	VAL	2.7
1	E	131	ASP	2.7
1	A	58	LYS	2.6
3	O	18	GLU	2.6
3	L	15	TYR	2.6
1	A	120	ARG	2.5
2	B	780	ILE	2.5
3	P	90	GLU	2.5
3	O	57	ASN	2.5
3	G	8	LEU	2.5
2	J	780	ILE	2.4
3	O	16	LEU	2.4
3	O	59	THR	2.4
3	G	62	LEU	2.4
3	L	13	GLN	2.4
3	O	69	ALA	2.4
1	E	45	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	K	61	ILE	2.3
2	F	766	ARG	2.3
3	P	89	LEU	2.3
3	O	32	ARG	2.3
1	M	102	PHE	2.2
3	K	50	MET	2.2
3	G	39	VAL	2.2
2	F	769	TYR	2.2
2	B	795	LYS	2.2
1	A	115	ILE	2.2
1	A	123	LYS	2.2
1	A	130	THR	2.2
3	C	61	ILE	2.1
1	A	137	MET	2.1
1	E	121	VAL	2.1
2	B	777	LEU	2.1
2	J	777	LEU	2.1
3	H	89	LEU	2.1
3	K	70	LEU	2.1
1	A	102	PHE	2.1
3	G	25	ILE	2.1
3	O	72	MET	2.1
1	A	118	LEU	2.0
3	K	77	THR	2.0
1	M	116	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
4	SO4	M	162	5/5	0.91	0.20	-0.17	104,115,124,128	0
4	SO4	A	162	5/5	0.96	0.15	-1.18	96,111,114,115	0
4	SO4	G	97	5/5	0.91	0.14	-1.27	135,141,141,141	0
4	SO4	I	162	5/5	0.95	0.16	-1.32	85,100,122,124	0

6.5 Other polymers [i](#)

There are no such residues in this entry.