



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:18 PM UTC

PDB ID : 3FWC / pdb_00003fwc
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

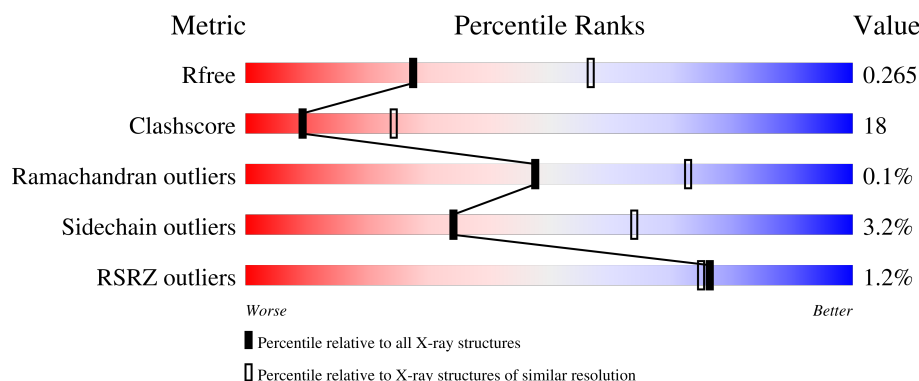
1 Overall quality at a glance

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.



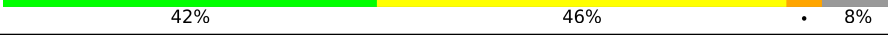
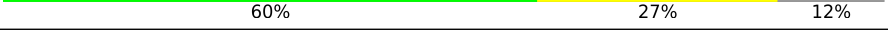
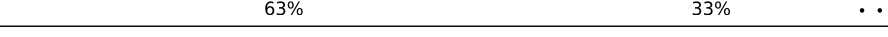
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	2% 58% 32% 10%
1	E	161	% 61% 29% 7%
1	I	161	75% 17% 9%
1	M	161	% 63% 27% 8%
2	B	85	67% 28% ...

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Mol	Chain	Length	Quality of chain
2	F	85	 67% 29% ..
2	J	85	 71% 21% 8%
2	N	85	 74% 24% ..
3	C	96	 64% 27% 9%
3	D	96	 67% 21% • 10%
3	G	96	 42% 46% • 8%
3	H	96	 60% 35% •
3	K	96	 36% 49% 5% • 8%
3	L	96	 60% 27% 12%
3	O	96	 43% 47% • • 7%
3	P	96	 63% 33% • •

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			

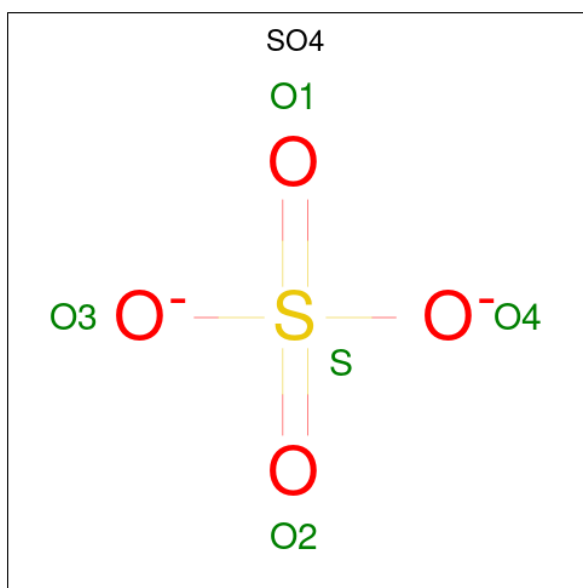
There are 8 discrepancies between the modelled and reference sequences:

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 (CCD ID: 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		

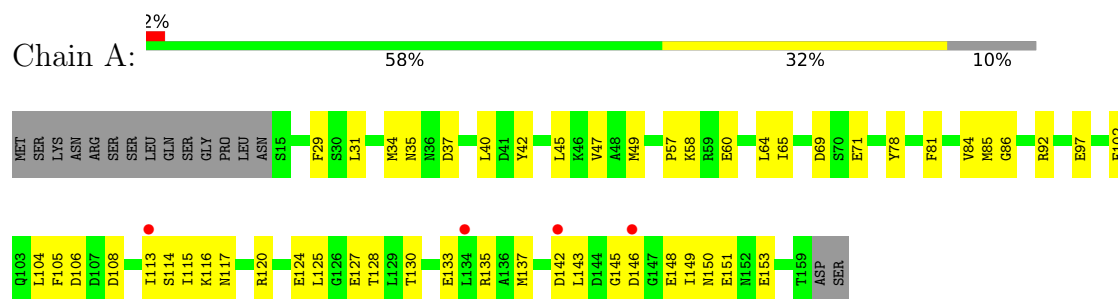
- Molecule 5 is water.

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		

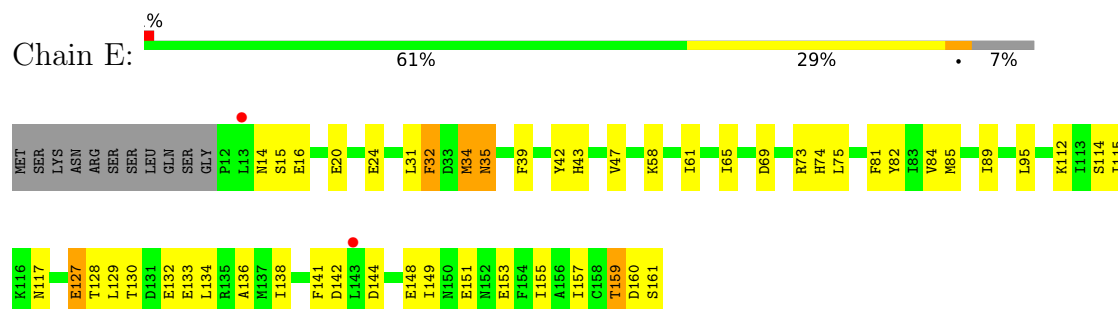
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

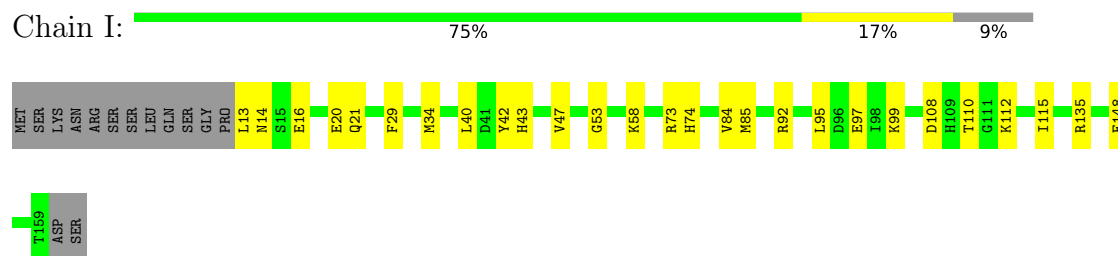
• Molecule 1: Cell division control protein 31



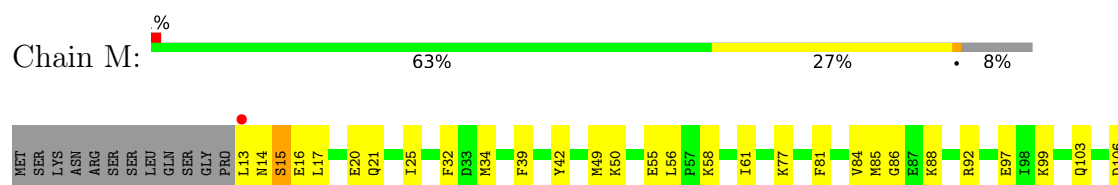
• Molecule 1: Cell division control protein 31



• Molecule 1: Cell division control protein 31



• Molecule 1: Cell division control protein 31





- Molecule 2: Nuclear mRNA export protein SAC3

Chain B: 67% 28% ...



- Molecule 2: Nuclear mRNA export protein SAC3

Chain F: 67% 29% ..



- Molecule 2: Nuclear mRNA export protein SAC3

Chain J: 71% 21% 8%



- Molecule 2: Nuclear mRNA export protein SAC3

Chain N: 74% 24% ..



- Molecule 3: Protein SUS1

Chain C: 64% 27% 9%



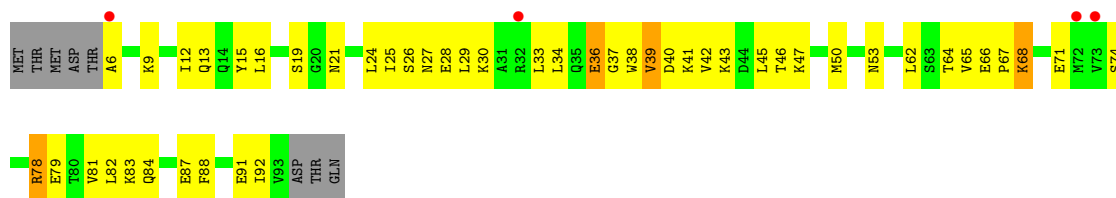
- Molecule 3: Protein SUS1

Chain D: 67% 21% 10%



- Molecule 3: Protein SUS1

Chain G: 42% 46% 8%



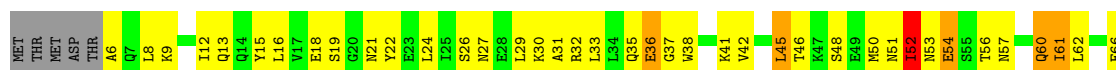
• Molecule 3: Protein SUS1

Chain H: 60% 35%



• Molecule 3: Protein SUS1

Chain K: 2% 36% 49% 5% 8%



• Molecule 3: Protein SUS1

Chain L: 60% 27% 12%



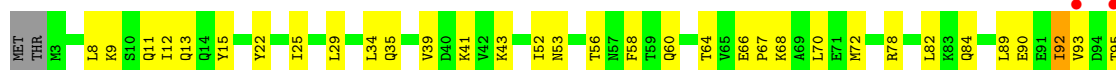
• Molecule 3: Protein SUS1

Chain O: 43% 47% 7%



• Molecule 3: Protein SUS1

Chain P: 2% 63% 33%



GLN

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 19.92 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.92-2.70) 98.6 (19.92-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.61Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.211 , 0.265 0.211 , 0.265	Depositor DCC
R_{free} test set	3470 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtrriage
Anisotropy	0.021	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 86.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13510	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtrriage'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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.39	0/1215	0.75	0/1628
1	E	0.43	0/1252	0.77	0/1679
1	I	0.45	0/1231	0.71	0/1650
1	M	0.47	0/1239	0.81	3/1661 (0.2%)
2	B	0.47	0/713	0.76	1/955 (0.1%)
2	F	0.47	0/719	0.72	0/963
2	J	0.50	0/673	0.70	0/901
2	N	0.59	0/719	0.69	0/963
3	C	0.42	0/713	0.77	0/960
3	D	0.42	0/703	0.79	2/946 (0.2%)
3	G	0.38	0/718	0.93	2/967 (0.2%)
3	H	0.43	0/749	0.77	0/1009
3	K	0.42	0/718	0.83	0/967
3	L	0.38	0/689	0.73	0/927
3	O	0.42	0/726	0.96	3/978 (0.3%)
3	P	0.49	0/756	0.78	0/1019
All	All	0.45	0/13533	0.78	11/18173 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	93	VAL	N-CA-C	9.56	119.51	110.53
2	B	725	VAL	N-CA-C	-7.01	104.59	113.22
3	D	55	SER	N-CA-C	-6.83	105.56	114.04
1	M	15	SER	N-CA-C	-6.71	101.67	110.33
3	O	53	ASN	N-CA-C	-5.84	105.47	112.59
3	O	54	GLU	N-CA-C	-5.56	105.83	113.56
3	G	37	GLY	N-CA-C	-5.36	106.83	115.08
3	G	82	LEU	N-CA-C	-5.31	105.39	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	86	GLY	N-CA-C	-5.28	106.38	112.50
1	M	81	PHE	N-CA-C	-5.13	106.28	112.54
3	D	9	LYS	N-CA-C	-5.11	105.90	111.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	42	0
1	E	1233	0	1187	54	0
1	I	1213	0	1173	19	0
1	M	1221	0	1177	33	0
2	B	702	0	711	39	0
2	F	708	0	716	24	0
2	J	662	0	663	22	0
2	N	708	0	716	22	0
3	C	707	0	718	28	0
3	D	697	0	703	23	0
3	G	712	0	723	52	0
3	H	743	0	747	21	0
3	K	712	0	723	78	0
3	L	683	0	690	20	0
3	O	720	0	727	45	0
3	P	750	0	754	27	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	475	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 18.

All (475) 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
3:K:51:ASN:HA	3:K:52:ILE:C	2.01	0.85
1:M:159:THR:O	1:M:160:ASP:HB2	1.79	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
2:B:782:MET:HA	2:B:782:MET:HE2	1.64	0.78
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:N	3:K:52:ILE:HD13	2.03	0.73
3:G:33:LEU:HD13	3:G:38:TRP:CE3	2.24	0.72
2:J:782:MET:HE2	2:J:782:MET:HA	1.72	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:34:MET:HE2	2:N:782:MET:SD	2.32	0.69
1:E:155:ILE:O	1:E:159:THR:HB	1.93	0.69
3:G:38:TRP:CE2	3:G:42:VAL:CG2	2.75	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
1:M:49:MET:HE1	1:M:61:ILE:HG12	1.77	0.67
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
2:B:785:ARG:HG2	3:C:50:MET:HE1	1.78	0.66
3:C:61:ILE:O	3:C:65:VAL:HG22	1.96	0.66
3:K:52:ILE:HD13	3:K:52:ILE:H	1.61	0.66
2:B:773:LEU:HD12	3:C:29:LEU:HD21	1.78	0.66
3:G:39:VAL:HG22	3:G:40:ASP:N	2.10	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
1:A:34:MET:CE	2:B:782:MET:HE1	2.26	0.65
3:P:8:LEU:O	3:P:12:ILE:HG12	1.97	0.65
3:K:29:LEU:O	3:K:33:LEU:HG	1.97	0.65
2:J:764:MET:HE1	3:K:12:ILE:HB	1.78	0.64
3:G:78:ARG:O	3:G:81:VAL:HG12	1.97	0.64
1:E:74:HIS:C	1:E:75:LEU:HD12	2.23	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
1:A:34:MET:HE3	2:B:782:MET:HE1	1.81	0.63
3:L:9:LYS:O	3:L:12:ILE:HG22	1.99	0.63
2:F:785:ARG:HD2	3:G:50:MET:HE3	1.80	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:P:41:LYS:HB3	3:P:72:MET:HE1	1.80	0.61
3:C:49:GLU:O	3:C:52:ILE:HG22	2.00	0.61
3:K:54:GLU:O	3:K:54:GLU:HG3	2.01	0.61
3:G:34:LEU:HD12	3:G:39:VAL:HG11	1.78	0.61
3:K:79:GLU:OE1	3:K:79:GLU:HA	2.01	0.61
1:A:102:PHE:CE2	1:A:151:GLU:HB2	2.35	0.61
1:E:75:LEU:HD12	1:E:75:LEU:N	2.15	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:B:799:PHE:C	2:B:799:PHE:CD2	2.79	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
2:F:734:LEU:HD12	3:H:22:TYR:CE1	2.36	0.59
3:K:46:THR:O	3:K:50:MET:HG3	2.02	0.59
3:O:93:VAL:HG23	3:O:94:ASP:C	2.27	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:A:71:GLU:HA	1:A:71:GLU:OE1	2.03	0.59
2:B:760:PHE:CE2	2:B:764:MET:HE2	2.37	0.59
2:J:776:ARG:NH2	3:K:30:LYS:HE2	2.18	0.59
1:A:133:GLU:O	1:A:137:MET:HG3	2.02	0.59
2:J:734:LEU:HD13	3:L:22:TYR:CZ	2.38	0.59
1:I:115:ILE:HD13	1:I:135:ARG:NH2	2.17	0.59
1:M:92:ARG:HD3	1:M:97:GLU:CD	2.28	0.58
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
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:51:ASN:CA	3:K:52:ILE:C	2.76	0.58
1:A:65:ILE:O	1:A:69:ASP:HB2	2.03	0.58
3:K:52:ILE:HG12	3:K:54:GLU:CB	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:ILE:HG23	3:C:52:ILE:O	2.03	0.58
1:E:161:SER:HA	2:F:801:LYS:NZ	2.18	0.58
3:G:78:ARG:CD	3:G:78:ARG:C	2.77	0.57
1:E:138:ILE:O	1:E:142:ASP:HB2	2.04	0.57
3:G:83:LYS:O	3:G:87:GLU:HB3	2.03	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:HG22	3:P:95:THR:O	2.05	0.57
1:E:42:TYR:OH	1:E:58:LYS:HG2	2.04	0.57
1:M:84:VAL:HG12	1:M:85:MET:HE2	1.87	0.57
3:O:70:LEU:O	3:O:73:VAL:HG12	2.05	0.57
1:E:34:MET:HE2	1:E:34:MET:HA	1.86	0.56
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:92:ARG:HD3	1:A:97:GLU:OE2	2.06	0.56
1:A:143:LEU:O	1:A:143:LEU:HD12	2.06	0.56
3:O:66:GLU:N	3:O:67:PRO:HD2	2.21	0.55
2:B:749:ARG:HH21	3:D:43:LYS:CE	2.20	0.55
1:M:106:ASP:OD1	1:M:112:LYS:O	2.24	0.55
2:B:781:TYR:HD2	2:B:782:MET:HE3	1.72	0.55
2:B:785:ARG:HD3	3:C:50:MET:HE1	1.89	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
2:B:725:VAL:HG22	2:B:728:GLU:CD	2.32	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
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
3:G:87:GLU:O	3:G:91:GLU:OE1	2.25	0.54
1:E:32:PHE:CD1	1:E:32:PHE:N	2.75	0.54
3:G:36:GLU:C	3:G:36:GLU:OE1	2.51	0.54
3:G:38:TRP:CZ2	3:G:42:VAL:HG21	2.42	0.54
3:L:83:LYS:O	3:L:87:GLU:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:75:ASP:O	3:O:79:GLU:HG2	2.08	0.54
3:G:78:ARG:C	3:G:78:ARG:HD3	2.32	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
2:J:785:ARG:HH21	3:K:50:MET:HE3	1.72	0.54
2:B:781:TYR:CD2	2:B:782:MET:HE3	2.43	0.53
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:O	1:E:128:THR:HG23	2.09	0.53
3:P:53:ASN:HB3	3:P:56:THR:OG1	2.08	0.53
1:I:34:MET:CE	2:J:782:MET:HE1	2.39	0.53
1:M:149:ILE:HD12	2:N:802:TRP:CZ2	2.44	0.53
1:A:45:LEU:HD11	1:A:49:MET:HE3	1.91	0.53
3:O:78:ARG:O	3:O:82:LEU:HD12	2.09	0.53
3:C:33:LEU:HD13	3:C:38:TRP:CE3	2.44	0.53
3:G:33:LEU:HD22	3:G: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:A:128:THR:HG23	1:A:128:THR:O	2.10	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:120:ARG:O	1:A:124:GLU:HB2	2.10	0.52
3:G:27:ASN:HA	3:G:30:LYS:HE3	1.91	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
1:E:129:LEU:HD22	1:E:133:GLU:CD	2.35	0.51
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
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
1:E:114:SER:H	1:E:117:ASN:HB2	1.77	0.50
3:K:42:VAL:O	3:K:45:LEU:HD12	2.10	0.50
3:L:73:VAL:O	3:L:73:VAL:HG23	2.10	0.50
2:N:761:ILE:HD11	3:O:93:VAL:HG21	1.94	0.50
3:H:12:ILE:HD13	3:H:89:LEU:HD11	1.93	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
2:B:785:ARG:CG	3:C:50:MET:HE1	2.42	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:G:68:LYS:O	3:G:71:GLU:HG2	2.11	0.49
3:K:15:TYR:O	3:K:19:SER:CB	2.60	0.49
3:G:64:THR:O	3:G:68:LYS:HE3	2.12	0.49
3:O:50:MET:HE2	3:O:50:MET:O	2.13	0.49
3:O:88:PHE:O	3:O:92:ILE:CD1	2.60	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
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
3:O:15:TYR:C	3:O:15:TYR:CD2	2.90	0.49
2:B:726:ILE:HG23	2:B:727:THR:N	2.28	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
3:K:38:TRP:O	3:K:42:VAL:HG23	2.12	0.49
3:K:53:ASN:O	3:K:54:GLU:C	2.55	0.49
3:D:58:PHE:HB2	1:I:13:LEU:HD23	1.93	0.49
1:E:34:MET:HA	1:E:34:MET:CE	2.43	0.49
1:E:69:ASP:OD2	1:E:73:ARG:O	2.30	0.49
1:I:13:LEU:HB3	1:I:14:ASN:CA	2.43	0.49
3:D:8:LEU:HD13	3:D:11:GLN:NE2	2.28	0.49
3:H:92:ILE:O	3:H:92:ILE:HG22	2.12	0.49
3:K:66:GLU:N	3:K:67:PRO:HD2	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:ILE:O	3:C:13:GLN:C	2.55	0.48
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:N:785:ARG:HD3	3:O:50:MET:HE1	1.94	0.48
1:A:34:MET:HE1	2:B:782:MET:HE1	1.95	0.48
2:B:727:THR:HG22	3:D:82:LEU:HD11	1.94	0.48
2:B:764:MET:HE1	3:C:12:ILE:HG13	1.94	0.48
3:K:41:LYS:CB	3:K:72:MET:HE1	2.44	0.48
1:E:130:THR:HG21	3:O:18:GLU:OE1	2.13	0.48
3:K:52:ILE:H	3:K:52:ILE:CD1	2.25	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
1:A:35:ASN:OD1	1:A:37:ASP:CG	2.57	0.48
1:A:106:ASP:HB2	1:A:113:ILE:CD1	2.43	0.48
3:O:74:SER:OG	3:O:77:THR:HG23	2.13	0.48
3:D:73:VAL:HG23	3:D:73:VAL:O	2.12	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
2:B:785:ARG:CD	3:C:50:MET:HE1	2.44	0.48
1:M:152:ASN:OD1	1:M:152:ASN:N	2.46	0.48
2:B:791:ASN:HB3	2:B:795:LYS:HE3	1.96	0.47
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
3:O:35:GLN:C	3:O:37:GLY:H	2.22	0.47
3:C:62:LEU:C	3:C:62:LEU:HD23	2.39	0.47
1:E:141:PHE:HZ	2:F:805:SER:CB	2.28	0.47
3:K:52:ILE:HG13	3:K:54:GLU:CD	2.39	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
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:P:53:ASN:CB	3:P:56:THR:OG1	2.63	0.47
2:B:781:TYR:OH	2:B:785:ARG:NH1	2.47	0.47
3:H:94:ASP:C	3:H:94:ASP:OD1	2.57	0.47
1:I:20:GLU:HG3	1:I:21:GLN:N	2.28	0.47
3:K:6:ALA:C	3:K:8:LEU:N	2.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:52:ILE:O	3:K:54:GLU:HB3	2.14	0.47
2:N:757:ARG:HH21	3:O:90:GLU:HG3	1.78	0.47
3:K:66:GLU:HB3	3:K:67:PRO:CD	2.43	0.47
1:M:14:ASN:HB3	1:M:15:SER:O	2.14	0.47
2:J:764:MET:HE3	3:K:9:LYS:HB3	1.96	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
2:F:722:SER:O	2:F:726:ILE:HG12	2.15	0.46
3:O:18:GLU:C	3:O:18:GLU:CD	2.83	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
3:H:61:ILE:O	3:H:65:VAL:HG23	2.15	0.46
1:I:34:MET:HE3	2:J:782:MET:HE1	1.96	0.46
3:K:89:LEU:O	3:K:93:VAL:HG23	2.16	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
1:E:115:ILE:HD11	1:E:134:LEU:HB2	1.96	0.46
2:J:730:ILE:HB	3:L:85:ILE:CD1	2.46	0.46
3:K:52:ILE:HG12	3:K:54:GLU:HB3	1.96	0.46
1:A:34:MET:HE3	2:B:782:MET:SD	2.55	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
3:P:92:ILE:CG2	3:P:93:VAL:N	2.76	0.46
1:E:84:VAL:HG12	1:E:85:MET:HE2	1.97	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:K:41:LYS:HB3	3:K:72:MET:HE1	1.97	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
2:F:731:ALA:O	2:F:735:VAL:HG23	2.15	0.46
2:J:735:VAL:O	2:J:739:VAL:HG12	2.16	0.46
3:K:75:ASP:O	3:K:79:GLU:HG2	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
2:F:781:TYR:CE2	3:G:62:LEU:HB2	2.51	0.45
3:K:22:TYR:C	3:K:22:TYR:CD2	2.94	0.45
3:K:83:LYS:O	3:K:87:GLU:HG3	2.16	0.45
2:F:776:ARG:HH12	2:F:779:LEU:HD12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:51:ASN:O	3:H:52:ILE:C	2.60	0.45
2:J:730:ILE:HD11	3:L:13:GLN:HB2	1.97	0.45
3:O:33:LEU:HB3	3:O:38:TRP:CE3	2.51	0.45
1:A:31:LEU:HD11	2:B:785:ARG:HE	1.82	0.45
3:H:53:ASN:C	3:H:55:SER:H	2.25	0.45
2:J:747:VAL:HG12	3:L:58:PHE:CE1	2.52	0.45
1:M:92:ARG:HD3	1:M:97:GLU:CG	2.46	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:G:12:ILE:HA	3:G:15:TYR:HB3	1.99	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
1:I:84:VAL:HG12	1:I:85:MET:HE2	1.98	0.45
3:K:45:LEU:HD12	3:K:45:LEU:N	2.32	0.45
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
1:A:34:MET:HE3	2:B:782:MET:CE	2.45	0.44
2:B:725:VAL:HG22	2:B:728:GLU:OE2	2.17	0.44
3:G:66:GLU:N	3:G:67:PRO:HD3	2.31	0.44
1:M:56:LEU:HD11	1:M:88:LYS:HE2	1.98	0.44
1:M:128:THR:HG22	1:M:128:THR:O	2.17	0.44
1:A:145:GLY:HA2	1:A:146:ASP:HA	1.66	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:K:30:LYS:O	3:K:31:ALA:C	2.61	0.44
3:O:8:LEU:O	3:O:12:ILE:HG12	2.17	0.44
3:P:64:THR:O	3:P:68:LYS:HD2	2.18	0.44
1:E:112:LYS:HD2	1:E:148:GLU:OE1	2.17	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:A:35:ASN:HB2	1:E:35:ASN:O	2.18	0.44
3:G:66:GLU:N	3:G:67:PRO:CD	2.81	0.44
3:H:63:SER:O	3:H:67:PRO:HD2	2.18	0.44
1:E:161:SER:HA	2:F:801:LYS:HZ1	1.80	0.44
1:M:15:SER:HA	1:M:17:LEU:N	2.33	0.44
1:A:104:LEU:HD21	2:B:791:ASN:ND2	2.32	0.44
3:K:41:LYS:HD3	3:K:72:MET:HE3	2.00	0.44
3:P:56:THR:CG2	3:P:60:GLN:HB2	2.48	0.44
2:B:752:SER:O	2:B:756:TYR:CD2	2.71	0.44
1:E:32:PHE:N	1:E:32:PHE:HD1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:724:GLN:HA	2:N:724:GLN:OE1	2.18	0.43
3:P:52:ILE:HG13	3:P:53:ASN:N	2.33	0.43
3:G:34:LEU:HD12	3:G:34:LEU:HA	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:N:728:GLU:O	2:N:729:GLN:C	2.60	0.43
2:F:764:MET:HE3	2:F:764:MET:HB3	1.75	0.43
3:G:84:GLN:O	3:G:87:GLU:HG2	2.19	0.43
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:G:19:SER:C	3:G:21:ASN:H	2.25	0.43
3:K:38:TRP:CE2	3:K:42:VAL:HG21	2.54	0.43
2:B:742:SER:O	2:B:746:ILE:HG13	2.19	0.43
3:D:12:ILE:N	3:D:12:ILE:CD1	2.80	0.43
2:B:727:THR:HG22	3:D:82:LEU:CD1	2.49	0.43
2:F:750:GLU:OE1	3:H:47:LYS:HE3	2.19	0.43
3:H:29:LEU:O	3:H:30:LYS:C	2.61	0.43
3:H:38:TRP:CZ2	3:H:42:VAL:HG21	2.54	0.43
3:K:6:ALA:HA	5:K:100:HOH:O	2.19	0.43
3:L:38:TRP:O	3:L:42:VAL:HG23	2.19	0.43
1:E:20:GLU:O	1:E:24:GLU:HG3	2.19	0.43
1:I:53:GLY:N	2:J:790:ARG:HD3	2.34	0.43
3:K:52:ILE:HG13	3:K:54:GLU:HB2	2.00	0.43
1:A:125:LEU:C	1:A:127:GLU:H	2.27	0.42
3:K:32:ARG:HH21	3:K:77:THR:HG22	1.83	0.42
3:K:50:MET:HE2	3:K:50:MET:HB3	1.81	0.42
3:K:54:GLU:O	3:K:54:GLU:CG	2.62	0.42
3:D:21:ASN:O	3:D:25:ILE:HG13	2.19	0.42
2:F:750:GLU:OE2	2:F:750:GLU:HA	2.19	0.42
3:G:46:THR:HG23	3:G:65:VAL:HG11	2.01	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
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:K:29:LEU:O	3:K:33:LEU:CG	2.66	0.42
3:O:92:ILE:HD12	3:O:92:ILE:N	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:16:LEU:HD13	3:G:88:PHE:CE2	2.54	0.42
3:K:79:GLU:OE1	3:K:79:GLU:CA	2.67	0.42
2:B:749:ARG:HH21	3:D:43:LYS:NZ	2.18	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
1:E:127:GLU:CA	1:E:127:GLU:OE1	2.67	0.42
3:K:51:ASN:HA	3:K:53:ASN:N	2.33	0.42
3:P:35:GLN:HB2	5:P:102:HOH:O	2.18	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
3:D:16:LEU:HD23	3:D:22:TYR:HD1	1.84	0.42
3:G:26:SER:O	3:G:30:LYS:HG3	2.19	0.42
1:I:34:MET:HE1	2:J:782:MET:HE1	2.02	0.42
1:M:149:ILE:HD12	2:N:802:TRP:CH2	2.54	0.42
2:N:727:THR:HG22	3:P:82:LEU:HD12	2.02	0.42
3:P:90:GLU:OE2	3:P:90:GLU:HA	2.20	0.42
1:A:85:MET:O	1:A:86:GLY:C	2.63	0.42
1:A:116:LYS:HG3	1:A:117:ASN:N	2.34	0.42
3:C:53:ASN:O	3:C:54:GLU:HB2	2.20	0.42
1:I:108:ASP:CG	1:I:110:THR:HG23	2.45	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
1:E:141:PHE:CD2	1:E:157:ILE:HG12	2.54	0.41
2:J:739:VAL:HG13	2:J:740:ASN:N	2.35	0.41
3:K:57:ASN:H	3:K:60:GLN:HG3	1.84	0.41
1:A:150:ASN:CG	1:A:153:GLU:HG3	2.45	0.41
2:F:723:LYS:O	2:F:727:THR:HG23	2.21	0.41
2:F:788:LEU:CD1	3:G:47:LYS:HE3	2.50	0.41
2:N:785:ARG:HH11	3:O:50:MET:HE1	1.85	0.41
1:E:32:PHE:CE2	1:E:47:VAL:HG12	2.55	0.41
3:G:6:ALA:N	3:G:9:LYS:HD2	2.35	0.41
2:J:728:GLU:CA	3:L:82:LEU:HD21	2.50	0.41
3:K:66:GLU:O	3:K:67:PRO:C	2.63	0.41
1:E:142:ASP:OD1	1:E:144:ASP:CB	2.68	0.41
1:I:95:LEU:O	1:I:99:LYS:HG3	2.21	0.41
3:O:16:LEU:HD12	3:O:21:ASN:HB3	2.01	0.41
3:O:41:LYS:HB3	3:O:72:MET:HE1	2.01	0.41
1:A:29:PHE:CE1	1:A:40:LEU:HG	2.55	0.41
1:A:115:ILE:HD13	1:A:135:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:G:27:ASN:OD1	3:G:28:GLU:HG3	2.20	0.41
3:K:29:LEU:HG	3:K:33:LEU:CD1	2.50	0.41
1:A:142:ASP:HB3	1:A:149:ILE:CD1	2.47	0.41
1:A:150:ASN:O	1:A:153:GLU:HB2	2.20	0.41
3:K:74:SER:OG	3:K:77:THR:HG23	2.21	0.41
3:L:26:SER:O	3:L:30:LYS:HG3	2.20	0.41
1:M:32:PHE:CZ	2:N:786:ALA:HB2	2.55	0.41
2:N:727:THR:HG22	3:P:82:LEU:CD1	2.51	0.41
1:A:29:PHE:CG	1:A:78:TYR:HD1	2.39	0.41
1:E:43:HIS:O	1:E:47:VAL:HG23	2.21	0.41
3:G:9:LYS:O	3:G:13:GLN:CB	2.69	0.41
3:G:71:GLU:OE1	3:G:71:GLU:HA	2.20	0.41
3:H:66:GLU:HB2	3:H:67:PRO:CD	2.50	0.41
3:O:36:GLU:OE2	3:O:77:THR:HG21	2.21	0.41
3:P:25:ILE:HG23	3:P:84:GLN:OE1	2.21	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
3:O:31:ALA:O	3:O:35:GLN:HG3	2.20	0.41
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:E:159:THR:CG2	1:E:160:ASP:N	2.80	0.40
1:I:92:ARG:NH1	5:I:164:HOH:O	2.55	0.40
3:K:35:GLN:C	3:K:37:GLY:H	2.29	0.40
3:K:77:THR:O	3:K:81:VAL:HG23	2.21	0.40
3:C:91:GLU:O	3:C:91:GLU:HG3	2.20	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: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
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
2:N:802:TRP:CD1	2:N:802:TRP:C	2.98	0.40
3:O:33:LEU:HD13	3:O:38:TRP:CE3	2.56	0.40
3:C:33:LEU:HD13	3:C:38:TRP:CZ3	2.57	0.40
3:H:60:GLN:CD	3:H:60:GLN:H	2.29	0.40
1:I:43:HIS:O	1:I:47:VAL:HG22	2.21	0.40
1:M:115:ILE:HG12	1:M:138:ILE:HD12	2.02	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	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%)	5	13
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%)	48	73

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%)	127 (95%)	7 (5%)	21	47
1	I	132/145 (91%)	130 (98%)	2 (2%)	57	81
1	M	133/145 (92%)	128 (96%)	5 (4%)	29	58
2	B	78/79 (99%)	75 (96%)	3 (4%)	29	58
2	F	79/79 (100%)	77 (98%)	2 (2%)	42	71
2	J	73/79 (92%)	70 (96%)	3 (4%)	27	56
2	N	79/79 (100%)	75 (95%)	4 (5%)	21	48
3	C	83/91 (91%)	82 (99%)	1 (1%)	63	84
3	D	81/91 (89%)	81 (100%)	0	100	100
3	G	83/91 (91%)	77 (93%)	6 (7%)	13	32
3	H	87/91 (96%)	86 (99%)	1 (1%)	65	85
3	K	83/91 (91%)	76 (92%)	7 (8%)	10	26
3	L	80/91 (88%)	79 (99%)	1 (1%)	61	83
3	O	84/91 (92%)	80 (95%)	4 (5%)	23	50
3	P	88/91 (97%)	86 (98%)	2 (2%)	44	73
All	All	1507/1624 (93%)	1459 (97%)	48 (3%)	34	64

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	725	VAL
2	B	728	GLU
2	B	796	LYS
3	C	14	GLN
1	E	32	PHE
1	E	34	MET
1	E	35	ASN
1	E	89	ILE

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Mol	Chain	Res	Type
1	E	95	LEU
1	E	127	GLU
1	E	159	THR
2	F	763	THR
2	F	764	MET
3	G	36	GLU
3	G	39	VAL
3	G	43	LYS
3	G	53	ASN
3	G	68	LYS
3	G	78	ARG
3	H	19	SER
1	I	16	GLU
1	I	97	GLU
2	J	743	VAL
2	J	783	ASP
2	J	792	SER
3	K	18	GLU
3	K	36	GLU
3	K	45	LEU
3	K	52	ILE
3	K	60	GLN
3	K	61	ILE
3	K	78	ARG
3	L	19	SER
1	M	13	LEU
1	M	20	GLU
1	M	117	ASN
1	M	139	GLU
1	M	152	ASN
2	N	725	VAL
2	N	737	GLU
2	N	775	GLU
2	N	785	ARG
3	O	50	MET
3	O	51	ASN
3	O	90	GLU
3	O	93	VAL
3	P	13	GLN
3	P	92	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
3	D	21	ASN
3	G	60	GLN
2	J	774	HIS
3	K	21	ASN
3	L	21	ASN
3	O	21	ASN
3	P	7	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.25	0	6,6,6	0.05	0
4	SO4	M	162	-	4,4,4	0.24	0	6,6,6	0.14	0
4	SO4	G	97	-	4,4,4	0.24	0	6,6,6	0.10	0
4	SO4	I	162	-	4,4,4	0.23	0	6,6,6	0.09	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 [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	144/161 (89%)	0.05	4 (2%) 55 51	58, 104, 160, 189	0
1	E	150/161 (93%)	-0.02	2 (1%) 75 73	52, 92, 145, 175	0
1	I	147/161 (91%)	-0.50	0 100 100	42, 70, 110, 136	0
1	M	148/161 (91%)	-0.36	2 (1%) 73 72	36, 79, 131, 160	0
2	B	83/85 (97%)	-0.36	0 100 100	58, 86, 120, 155	0
2	F	84/85 (98%)	-0.21	0 100 100	59, 91, 121, 140	0
2	J	78/85 (91%)	-0.50	0 100 100	54, 70, 113, 146	0
2	N	84/85 (98%)	-0.56	0 100 100	31, 68, 98, 152	0
3	C	85/96 (88%)	-0.16	1 (1%) 76 75	66, 111, 160, 184	0
3	D	86/96 (89%)	-0.29	1 (1%) 76 75	56, 91, 137, 150	0
3	G	80/96 (83%)	0.60	4 (5%) 34 30	15, 150, 204, 220	1 (1%)
3	H	92/96 (95%)	-0.37	0 100 100	51, 90, 122, 173	0
3	K	87/96 (90%)	0.21	2 (2%) 61 58	61, 116, 157, 172	0
3	L	84/96 (87%)	-0.16	1 (1%) 76 75	70, 108, 159, 185	0
3	O	84/96 (87%)	0.18	0 100 100	75, 142, 171, 210	0
3	P	93/96 (96%)	-0.37	2 (2%) 62 59	37, 69, 145, 165	0
All	All	1609/1752 (91%)	-0.18	19 (1%) 76 75	15, 93, 160, 220	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	13	LEU	4.0
1	A	142	ASP	2.8
3	P	95	THR	2.8
3	C	8	LEU	2.8
3	K	69	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	6	ALA	2.6
1	E	143	LEU	2.5
3	P	93	VAL	2.5
3	L	92	ILE	2.4
3	G	73	VAL	2.4
3	G	6	ALA	2.4
3	G	72	MET	2.3
3	K	72	MET	2.3
1	M	13	LEU	2.2
1	A	113	ILE	2.1
1	A	146	ASP	2.1
1	A	134	LEU	2.1
1	M	115	ILE	2.1
3	G	32	ARG	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	G	97	5/5	0.79	0.13	135,141,141,141	0
4	SO4	A	162	5/5	0.88	0.07	96,111,114,115	0
4	SO4	I	162	5/5	0.88	0.08	85,100,122,124	0
4	SO4	M	162	5/5	0.94	0.06	104,115,124,128	0

6.5 Other polymers [i](#)

There are no such residues in this entry.