Full wwPDB X-ray Structure Validation Report (i)

Dec 6, 2023 – 05:37 am GMT

PDB ID	:	2V7D
Title	:	14-3-3 protein zeta in complex with Thr758 phosphorylated integrin beta2 peptide
Authors	:	Takala, H.; Ylanne, J.
Deposited on	:	2007-07-30
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

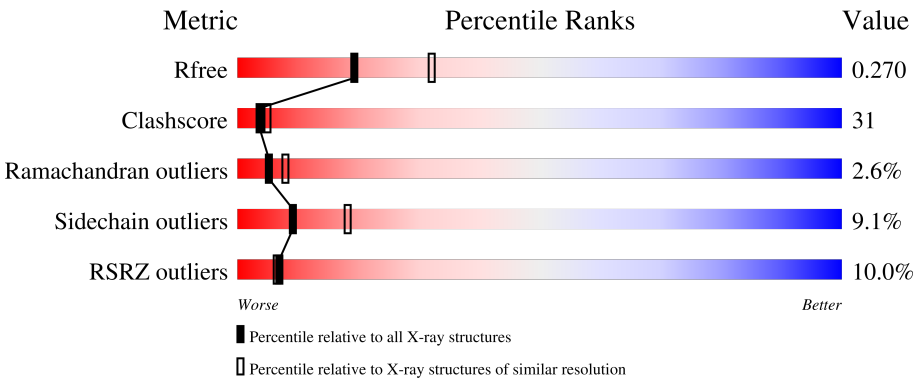
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	247	8%, 43%, 45%, 5%, 7%
1	B	247	10%, 42%, 44%, 6%, 8%
1	C	247	11%, 42%, 45%, 5%, 8%
1	D	247	9%, 44%, 43%, 5%, 8%
2	P	10	10%, 60%, 10%, 20%

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Mol	Chain	Length	Quality of chain
2	Q	10	10% 60% 10% 20%
2	R	10	20% 70% 10% 20%
2	S	10	10% 10% 60% 10% 20%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7645 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 14-3-3 PROTEIN ZETA/DELTA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	229	1827	1145	308	364	10	0	0	1
1	B	227	1816	1139	306	361	10	0	0	1
1	C	227	1816	1139	306	361	10	0	0	1
1	D	228	1819	1141	307	361	10	0	0	1

- Molecule 2 is a protein called INTEGRIN BETA CHAIN, BETA 2 VARIANT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	P	8	53	29	9	14	1	0	0	1
2	Q	8	53	29	9	14	1	0	0	1
2	R	8	53	29	9	14	1	0	0	1
2	S	8	53	29	9	14	1	0	0	1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	39	39	39	0	0
3	B	32	32	32	0	0
3	C	36	36	36	0	0
3	D	34	34	34	0	0

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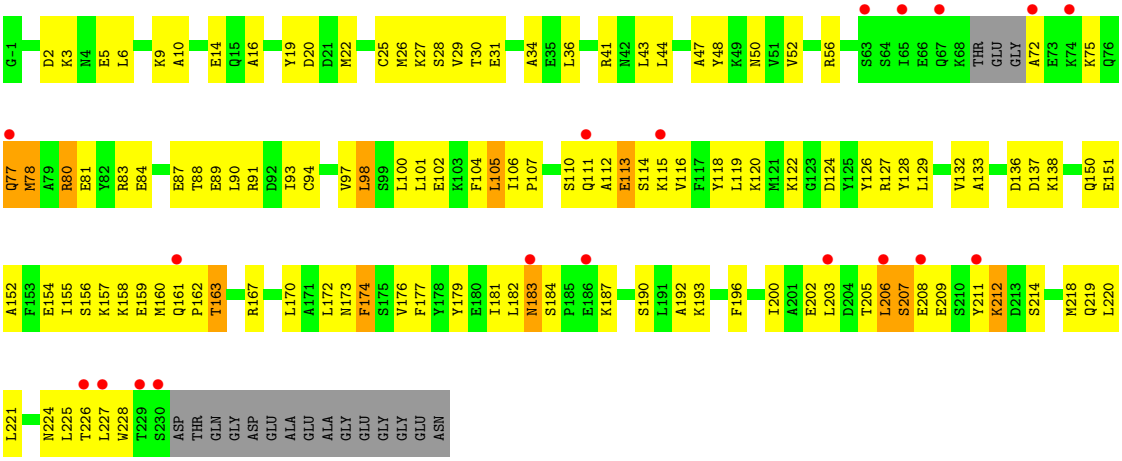
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	P	2	2	2	0	0
			Total	O		
3	Q	6	6	6	0	0
			Total	O		
3	R	3	3	3	0	0
			Total	O		
3	S	3	3	3	0	0

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.

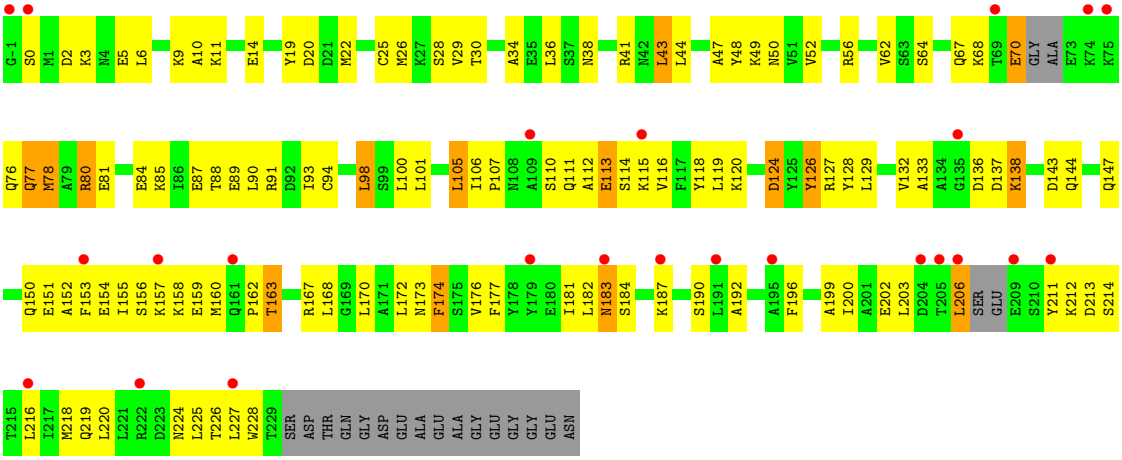
• Molecule 1: 14-3-3 PROTEIN ZETA/DELTA

Chain A:



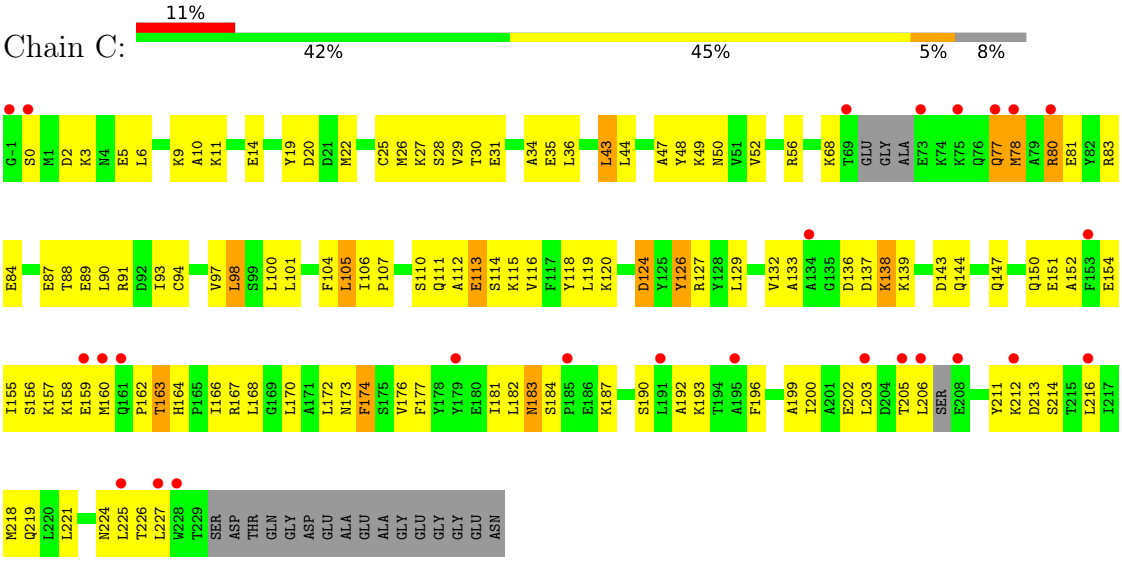
• Molecule 1: 14-3-3 PROTEIN ZETA/DELTA

Chain B:



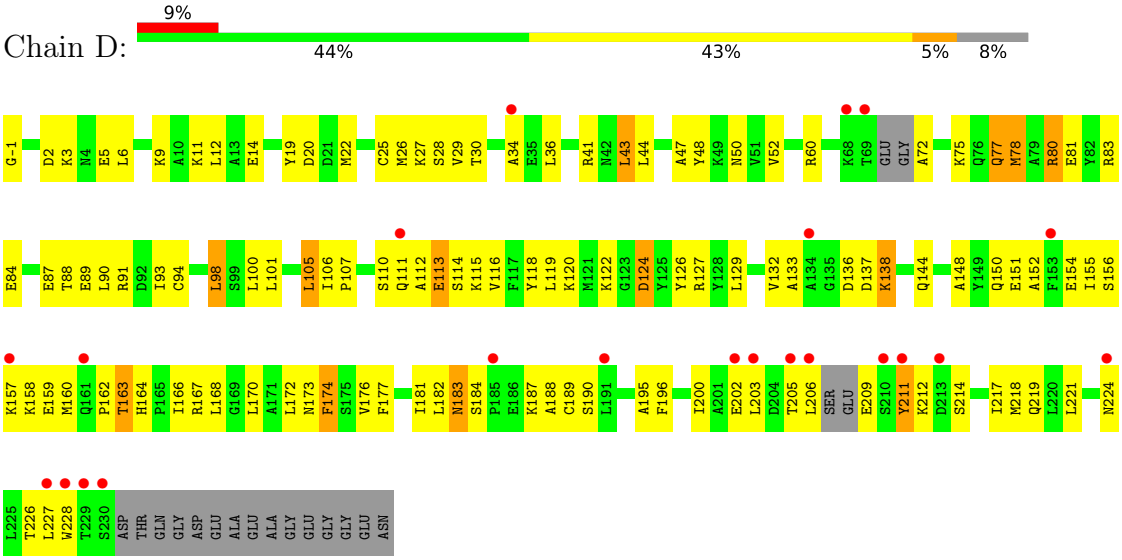
• Molecule 1: 14-3-3 PROTEIN ZETA/DELTA

Chain C:



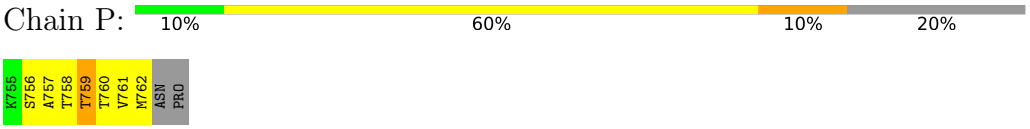
• Molecule 1: 14-3-3 PROTEIN ZETA/DELTA

Chain D:



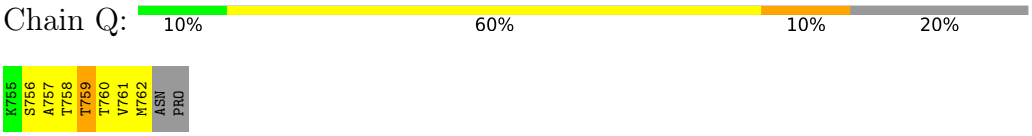
• Molecule 2: INTEGRIN BETA CHAIN, BETA 2 VARIANT

Chain P:



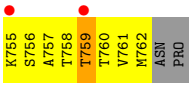
• Molecule 2: INTEGRIN BETA CHAIN, BETA 2 VARIANT

Chain Q:



• Molecule 2: INTEGRIN BETA CHAIN, BETA 2 VARIANT

Chain R:



- Molecule 2: INTEGRIN BETA CHAIN, BETA 2 VARIANT

Chain S:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	94.92Å 94.92Å 233.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.60 – 2.50 47.61 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.1 (47.60-2.50) 99.9 (47.61-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	4.59 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.228 , 0.273 0.226 , 0.270	Depositor DCC
R_{free} test set	1967 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 60.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.289 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7645	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: TPO

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	0.45	0/1851	0.60	0/2487
1	B	0.40	0/1839	0.57	0/2469
1	C	0.41	0/1839	0.59	0/2469
1	D	0.44	0/1842	0.59	1/2474 (0.0%)
2	P	0.76	0/40	0.58	0/52
2	Q	0.69	0/40	0.62	0/52
2	R	0.78	0/40	0.56	0/52
2	S	0.73	0/40	0.57	0/52
All	All	0.43	0/7531	0.59	1/10107 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	-1	GLY	N-CA-C	-5.32	99.81	113.10

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	1827	0	1819	117	0
1	B	1816	0	1808	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1816	0	1808	125	0
1	D	1819	0	1814	107	0
2	P	53	0	50	6	0
2	Q	53	0	50	8	0
2	R	53	0	50	11	0
2	S	53	0	50	8	0
3	A	39	0	0	5	0
3	B	32	0	0	6	0
3	C	36	0	0	2	0
3	D	34	0	0	5	0
3	P	2	0	0	0	0
3	Q	6	0	0	0	0
3	R	3	0	0	1	0
3	S	3	0	0	0	0
All	All	7645	0	7449	470	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 31.

All (470) 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:B:70:GLU:HA	1:B:76:GLN:NE2	1.42	1.31
1:B:203:LEU:HD23	1:B:206:LEU:HD11	1.41	0.99
1:B:70:GLU:CA	1:B:76:GLN:NE2	2.28	0.97
1:B:70:GLU:HA	1:B:76:GLN:HE21	1.07	0.87
1:D:72:ALA:HB1	1:D:75:LYS:HB3	1.57	0.87
1:C:192:ALA:HB3	1:C:225:LEU:HD21	1.60	0.83
1:B:0:SER:HB3	1:C:126:TYR:HE1	1.42	0.82
1:B:0:SER:HB3	1:C:126:TYR:CE1	2.15	0.81
1:A:105:LEU:HG	1:A:118:TYR:CE1	2.15	0.81
1:D:30:THR:HG21	1:D:100:LEU:HG	1.64	0.80
1:C:30:THR:HG21	1:C:100:LEU:HG	1.65	0.78
1:A:207:SER:O	1:A:209:GLU:N	2.18	0.77
1:C:90:LEU:HD13	1:C:132:VAL:HG11	1.66	0.77
1:A:87:GLU:HG2	1:A:91:ARG:NH2	2.00	0.76
1:B:87:GLU:HG2	1:B:91:ARG:NH2	2.01	0.75
1:A:91:ARG:NH1	3:A:2026:HOH:O	2.19	0.75
1:C:105:LEU:HG	1:C:118:TYR:CE1	2.21	0.75
1:C:87:GLU:HG2	1:C:91:ARG:NH2	2.01	0.75
1:D:87:GLU:HG2	1:D:91:ARG:NH2	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:LEU:HG	1:D:118:TYR:CE1	2.21	0.75
1:B:36:LEU:CD1	1:B:105:LEU:HD11	2.17	0.74
1:A:212:LYS:HB2	3:A:2037:HOH:O	1.87	0.74
1:C:176:VAL:HG13	2:R:756:SER:HB2	1.70	0.74
1:C:9:LYS:HG2	1:D:78:MET:CE	2.18	0.73
1:B:90:LEU:HD13	1:B:132:VAL:HG11	1.70	0.73
1:D:122:LYS:HE2	3:D:2027:HOH:O	1.87	0.72
1:A:90:LEU:HD13	1:A:132:VAL:HG11	1.70	0.72
1:D:80:ARG:HH11	1:D:80:ARG:HB2	1.54	0.72
1:A:196:PHE:CZ	1:A:200:ILE:HD11	2.23	0.72
1:C:129:LEU:O	1:C:133:ALA:HB2	1.89	0.72
1:B:41:ARG:HD3	3:B:2011:HOH:O	1.88	0.71
1:A:9:LYS:HG2	1:B:78:MET:CE	2.19	0.71
1:A:172:LEU:HD11	1:A:224:ASN:ND2	2.06	0.71
1:B:105:LEU:HG	1:B:118:TYR:CE1	2.25	0.71
1:B:129:LEU:O	1:B:133:ALA:HB2	1.90	0.71
1:B:67:GLN:O	1:B:70:GLU:CB	2.39	0.71
1:B:25:CYS:O	1:B:29:VAL:HG23	1.90	0.71
1:A:30:THR:HG23	1:A:105:LEU:HD13	1.71	0.71
1:A:25:CYS:O	1:A:29:VAL:HG23	1.90	0.70
1:D:90:LEU:HD13	1:D:132:VAL:HG11	1.72	0.70
1:C:196:PHE:CZ	1:C:200:ILE:HD11	2.27	0.70
1:D:173:ASN:HD21	2:S:759:THR:H	1.37	0.70
1:A:129:LEU:O	1:A:133:ALA:HB2	1.91	0.70
1:B:30:THR:HG21	1:B:100:LEU:HG	1.73	0.70
1:D:129:LEU:O	1:D:133:ALA:HB2	1.91	0.69
1:D:196:PHE:CZ	1:D:200:ILE:HD11	2.27	0.69
1:A:112:ALA:HA	1:A:115:LYS:HE3	1.74	0.69
1:D:25:CYS:O	1:D:29:VAL:HG23	1.92	0.69
1:C:36:LEU:CD1	1:C:105:LEU:HD11	2.23	0.68
1:C:106:ILE:HB	1:C:107:PRO:HD3	1.76	0.68
1:B:80:ARG:HH11	1:B:80:ARG:HB2	1.58	0.68
1:D:80:ARG:HH11	1:D:80:ARG:CB	2.06	0.68
1:D:2:ASP:OD2	1:D:5:GLU:HB2	1.94	0.67
1:B:196:PHE:CZ	1:B:200:ILE:HD11	2.28	0.67
1:B:36:LEU:HD11	1:B:105:LEU:HD11	1.75	0.67
1:C:80:ARG:HH11	1:C:80:ARG:HB2	1.60	0.67
1:C:172:LEU:HD11	1:C:224:ASN:ND2	2.10	0.67
1:A:30:THR:HG21	1:A:100:LEU:HG	1.76	0.66
1:D:112:ALA:HA	1:D:115:LYS:HE3	1.77	0.66
1:B:112:ALA:HA	1:B:115:LYS:HE3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ARG:HB2	1:A:80:ARG:HH11	1.60	0.66
1:A:207:SER:C	1:A:209:GLU:H	1.99	0.66
1:B:160:MET:HA	3:B:2029:HOH:O	1.95	0.66
1:D:115:LYS:O	1:D:119:LEU:HB2	1.97	0.66
1:B:70:GLU:HG2	1:B:76:GLN:HE22	1.59	0.65
1:B:176:VAL:HG13	2:Q:756:SER:HB2	1.77	0.65
1:C:49:LYS:HE2	3:R:2002:HOH:O	1.95	0.65
1:B:80:ARG:HH11	1:B:80:ARG:CB	2.10	0.65
1:C:25:CYS:O	1:C:29:VAL:HG23	1.97	0.65
1:B:41:ARG:HG3	1:B:118:TYR:OH	1.96	0.65
1:B:101:LEU:HD23	1:B:105:LEU:HD23	1.78	0.64
1:D:206:LEU:HB3	1:D:211:TYR:N	2.12	0.64
1:A:80:ARG:HH11	1:A:80:ARG:CB	2.10	0.64
1:C:80:ARG:HH11	1:C:80:ARG:CB	2.10	0.64
1:C:176:VAL:HG21	2:R:757:ALA:O	1.97	0.64
1:B:106:ILE:HB	1:B:107:PRO:HD3	1.80	0.64
1:A:106:ILE:HB	1:A:107:PRO:HD3	1.79	0.64
1:B:150:GLN:HE21	1:B:154:GLU:HG3	1.63	0.64
1:A:102:GLU:HG2	3:A:2032:HOH:O	1.97	0.64
1:C:6:LEU:HD13	1:C:28:SER:HB3	1.79	0.64
1:B:196:PHE:O	1:B:200:ILE:HG13	1.98	0.64
1:C:112:ALA:HA	1:C:115:LYS:HE3	1.80	0.64
1:B:44:LEU:CD2	1:B:105:LEU:HD21	2.28	0.63
1:C:127:ARG:HH22	2:R:758:TPO:P	2.21	0.63
1:A:36:LEU:HB2	1:A:118:TYR:OH	1.97	0.63
1:A:44:LEU:HD21	1:A:105:LEU:HD21	1.80	0.63
1:B:3:LYS:HE3	1:B:34:ALA:HB3	1.81	0.62
1:C:203:LEU:O	1:C:206:LEU:HG	1.99	0.62
1:B:80:ARG:O	1:B:84:GLU:HG3	2.00	0.62
1:C:56:ARG:HH22	2:R:755:LYS:HE2	1.63	0.62
1:A:36:LEU:CD1	1:A:105:LEU:HD11	2.29	0.62
1:C:78:MET:CE	1:D:9:LYS:HG2	2.28	0.62
1:C:150:GLN:HE21	1:C:154:GLU:HG3	1.64	0.62
1:A:9:LYS:HG2	1:B:78:MET:SD	2.40	0.61
1:B:176:VAL:HG21	2:Q:757:ALA:O	2.00	0.61
1:D:22:MET:HG2	1:D:47:ALA:HB2	1.82	0.61
1:A:36:LEU:HD11	1:A:105:LEU:HD11	1.81	0.61
1:A:196:PHE:O	1:A:200:ILE:HG13	2.00	0.61
1:A:101:LEU:HD23	1:A:105:LEU:HD23	1.82	0.61
1:D:106:ILE:HB	1:D:107:PRO:HD3	1.83	0.61
2:R:761:VAL:HG12	2:R:762:MET:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLN:HE21	1:A:163:THR:HG23	1.65	0.60
1:C:196:PHE:O	1:C:200:ILE:HG13	2.02	0.60
1:A:192:ALA:HB3	1:A:225:LEU:HD21	1.83	0.60
1:B:44:LEU:HD21	1:B:105:LEU:HD21	1.83	0.60
1:B:172:LEU:HD11	1:B:224:ASN:ND2	2.16	0.60
1:C:3:LYS:HE3	1:C:34:ALA:HB3	1.83	0.60
1:C:101:LEU:HD23	1:C:105:LEU:HD23	1.82	0.60
1:B:2:ASP:OD2	1:B:5:GLU:HB2	2.02	0.60
1:A:205:THR:O	1:A:206:LEU:C	2.40	0.60
1:A:172:LEU:O	1:A:176:VAL:HG23	2.02	0.59
1:D:158:LYS:O	1:D:159:GLU:HG2	2.02	0.59
2:S:761:VAL:HG12	2:S:762:MET:N	2.17	0.59
1:A:27:LYS:HA	1:A:100:LEU:HD21	1.84	0.59
1:B:115:LYS:O	1:B:119:LEU:HB2	2.03	0.59
2:Q:761:VAL:HG12	2:Q:762:MET:N	2.17	0.59
1:A:161:GLN:HE21	1:A:163:THR:CG2	2.14	0.59
1:C:158:LYS:O	1:C:159:GLU:HG2	2.02	0.59
1:C:2:ASP:OD2	1:C:5:GLU:HB2	2.03	0.59
1:A:78:MET:CE	1:B:9:LYS:HG2	2.32	0.59
1:D:200:ILE:O	1:D:203:LEU:HB2	2.03	0.58
1:C:113:GLU:HA	1:C:116:VAL:HG12	1.85	0.58
1:A:115:LYS:O	1:A:119:LEU:HB2	2.03	0.58
1:A:206:LEU:O	1:A:207:SER:C	2.41	0.58
1:B:6:LEU:HD13	1:B:28:SER:HB3	1.83	0.58
1:D:150:GLN:HE21	1:D:154:GLU:HG3	1.69	0.58
1:A:127:ARG:HG3	1:A:181:ILE:HG13	1.84	0.58
1:B:70:GLU:CA	1:B:76:GLN:HE21	1.99	0.58
1:D:101:LEU:HD23	1:D:105:LEU:HD23	1.84	0.58
1:A:200:ILE:O	1:A:203:LEU:HB2	2.03	0.58
1:B:158:LYS:O	1:B:159:GLU:HG2	2.03	0.58
1:A:3:LYS:HE3	1:A:34:ALA:HB3	1.85	0.58
1:C:203:LEU:HD23	1:C:206:LEU:CD1	2.33	0.58
1:D:80:ARG:O	1:D:84:GLU:HG3	2.02	0.58
1:C:80:ARG:O	1:C:84:GLU:HG3	2.04	0.58
1:D:196:PHE:O	1:D:200:ILE:HG13	2.04	0.58
1:D:36:LEU:CD1	1:D:105:LEU:HD11	2.34	0.57
1:A:80:ARG:O	1:A:84:GLU:HG3	2.03	0.57
1:A:150:GLN:HE21	1:A:154:GLU:HG3	1.69	0.57
1:B:64:SER:OG	1:B:68:LYS:HE2	2.05	0.57
1:C:115:LYS:O	1:C:119:LEU:HB2	2.04	0.57
1:B:120:LYS:HE2	1:B:173:ASN:ND2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LYS:HG2	1:A:157:LYS:O	2.05	0.57
1:B:67:GLN:O	1:B:70:GLU:HB2	2.04	0.56
1:C:56:ARG:NH2	2:R:755:LYS:HE2	2.20	0.56
1:B:200:ILE:O	1:B:203:LEU:HB2	2.05	0.56
1:D:127:ARG:NH2	2:S:758:TPO:HG21	2.20	0.56
1:D:206:LEU:HB3	1:D:211:TYR:H	1.68	0.56
1:A:44:LEU:CD2	1:A:105:LEU:HD21	2.34	0.56
1:A:158:LYS:O	1:A:159:GLU:HG2	2.05	0.56
1:C:36:LEU:HD11	1:C:105:LEU:HD11	1.86	0.56
1:C:200:ILE:O	1:C:203:LEU:HB2	2.05	0.56
1:D:182:LEU:O	1:D:184:SER:N	2.39	0.56
1:B:56:ARG:NH1	1:B:128:TYR:CE1	2.73	0.56
1:B:67:GLN:O	1:B:70:GLU:HB3	2.04	0.56
1:C:44:LEU:CD2	1:C:105:LEU:HD21	2.35	0.56
1:C:127:ARG:HG3	1:C:181:ILE:HG13	1.87	0.56
1:C:157:LYS:O	1:C:157:LYS:HG2	2.06	0.56
1:D:14:GLU:HB2	1:D:22:MET:SD	2.45	0.56
1:A:6:LEU:HD13	1:A:28:SER:HB3	1.87	0.56
1:B:203:LEU:HA	1:B:206:LEU:HD21	1.88	0.56
1:A:2:ASP:OD2	1:A:5:GLU:HB2	2.05	0.55
1:B:162:PRO:HG3	1:B:167:ARG:NH1	2.22	0.55
1:A:162:PRO:HG3	1:A:167:ARG:NH1	2.20	0.55
1:B:113:GLU:HA	1:B:116:VAL:HG12	1.89	0.55
1:D:172:LEU:HD11	1:D:224:ASN:ND2	2.22	0.55
1:A:172:LEU:HD11	1:A:224:ASN:HD21	1.72	0.55
1:D:6:LEU:HD13	1:D:28:SER:HB3	1.87	0.55
1:B:22:MET:HG2	1:B:47:ALA:HB2	1.89	0.55
1:C:203:LEU:HD23	1:C:206:LEU:HD11	1.87	0.55
1:C:77:GLN:O	1:C:81:GLU:HG3	2.07	0.55
1:A:22:MET:HG2	1:A:47:ALA:HB2	1.87	0.54
1:A:94:CYS:O	1:A:98:LEU:HB2	2.07	0.54
1:B:77:GLN:O	1:B:81:GLU:HG3	2.07	0.54
1:D:41:ARG:HG3	1:D:118:TYR:OH	2.06	0.54
2:Q:757:ALA:O	2:Q:758:TPO:HG22	2.08	0.54
1:A:30:THR:HG23	1:A:105:LEU:CD1	2.37	0.54
1:A:111:GLN:HB2	1:A:114:SER:OG	2.07	0.54
1:A:113:GLU:HA	1:A:116:VAL:HG12	1.89	0.54
1:A:176:VAL:HG21	2:P:757:ALA:O	2.08	0.54
1:C:48:TYR:O	1:C:52:VAL:HG12	2.07	0.54
1:D:113:GLU:HA	1:D:116:VAL:HG12	1.90	0.54
1:B:157:LYS:O	1:B:157:LYS:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:PRO:HG3	1:C:167:ARG:NH1	2.23	0.54
1:D:113:GLU:HB3	1:D:160:MET:HE3	1.89	0.54
1:A:113:GLU:HB3	1:A:160:MET:HE3	1.90	0.53
2:P:761:VAL:HG12	2:P:762:MET:N	2.23	0.53
1:C:22:MET:HG2	1:C:47:ALA:HB2	1.91	0.53
2:P:759:THR:HG22	2:P:760:THR:N	2.23	0.53
1:C:30:THR:HG23	1:C:105:LEU:HD13	1.89	0.53
1:D:127:ARG:HH22	2:S:758:TPO:HG21	1.72	0.53
1:D:188:ALA:HB1	1:D:228:TRP:CZ3	2.43	0.53
2:R:757:ALA:O	2:R:758:TPO:HG22	2.09	0.53
1:D:162:PRO:HG3	1:D:167:ARG:NH1	2.23	0.53
2:S:759:THR:HG22	2:S:760:THR:N	2.24	0.53
1:B:172:LEU:O	1:B:176:VAL:HG23	2.08	0.53
1:C:44:LEU:HD21	1:C:105:LEU:HD21	1.91	0.53
1:D:156:SER:C	1:D:158:LYS:H	2.13	0.53
1:B:156:SER:C	1:B:158:LYS:H	2.11	0.52
1:C:172:LEU:O	1:C:176:VAL:HG23	2.09	0.52
1:C:192:ALA:CB	1:C:225:LEU:HD21	2.38	0.52
1:D:3:LYS:HE3	1:D:34:ALA:HB3	1.91	0.52
1:D:113:GLU:CB	1:D:160:MET:HE3	2.39	0.52
1:A:207:SER:C	1:A:209:GLU:N	2.61	0.52
1:A:113:GLU:CB	1:A:160:MET:HE3	2.40	0.52
1:A:120:LYS:HE2	1:A:173:ASN:ND2	2.23	0.52
1:B:182:LEU:O	1:B:184:SER:N	2.42	0.52
1:A:156:SER:C	1:A:158:LYS:H	2.13	0.52
1:C:127:ARG:NH2	2:R:758:TPO:HG21	2.24	0.52
1:C:155:ILE:O	1:C:159:GLU:HB2	2.09	0.52
1:D:94:CYS:O	1:D:98:LEU:HB2	2.10	0.52
1:D:163:THR:CG2	1:D:202:GLU:HB2	2.40	0.51
2:Q:759:THR:HG22	2:Q:760:THR:N	2.24	0.51
1:B:132:VAL:HG13	3:B:2026:HOH:O	2.09	0.51
1:D:226:THR:C	1:D:228:TRP:H	2.14	0.51
1:C:170:LEU:O	1:C:174:PHE:HB2	2.10	0.51
1:D:80:ARG:HB2	1:D:80:ARG:NH1	2.23	0.51
1:A:163:THR:CG2	1:A:202:GLU:HB2	2.40	0.51
1:C:94:CYS:O	1:C:98:LEU:HB2	2.10	0.51
1:C:127:ARG:NH2	2:R:758:TPO:O1P	2.44	0.51
1:D:163:THR:HB	1:D:206:LEU:HD21	1.91	0.51
1:C:120:LYS:HE2	1:C:173:ASN:ND2	2.26	0.51
1:A:182:LEU:O	1:A:184:SER:N	2.43	0.51
1:D:155:ILE:O	1:D:159:GLU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:THR:HG21	1:D:202:GLU:HB2	1.93	0.51
1:D:174:PHE:O	1:D:177:PHE:HB3	2.11	0.51
1:A:226:THR:HG22	1:A:227:LEU:HD12	1.93	0.50
1:D:148:ALA:HB2	3:D:2027:HOH:O	2.10	0.50
1:A:127:ARG:HH22	2:P:758:TPO:P	2.34	0.50
1:B:127:ARG:HG3	1:B:181:ILE:HG13	1.93	0.50
1:C:163:THR:CG2	1:C:202:GLU:HB2	2.41	0.50
1:D:44:LEU:CD2	1:D:105:LEU:HD21	2.41	0.50
1:B:174:PHE:O	1:B:177:PHE:HB3	2.10	0.50
1:D:44:LEU:HD21	1:D:105:LEU:HD21	1.94	0.50
1:A:94:CYS:HB2	1:A:129:LEU:HD13	1.94	0.50
1:A:48:TYR:O	1:A:52:VAL:HG12	2.11	0.50
1:D:127:ARG:HG3	1:D:181:ILE:HG13	1.92	0.50
2:R:759:THR:HG22	2:R:760:THR:N	2.26	0.50
1:B:101:LEU:HA	1:B:105:LEU:HB2	1.91	0.50
1:C:172:LEU:CD1	1:C:224:ASN:ND2	2.75	0.50
1:A:206:LEU:C	1:A:207:SER:O	2.50	0.50
1:C:156:SER:C	1:C:158:LYS:H	2.15	0.50
1:D:77:GLN:O	1:D:81:GLU:HG3	2.11	0.50
1:D:176:VAL:HG13	2:S:756:SER:HB2	1.93	0.50
1:A:163:THR:HG21	1:A:202:GLU:HB2	1.94	0.50
1:D:172:LEU:O	1:D:176:VAL:HG23	2.12	0.50
1:C:174:PHE:O	1:C:177:PHE:HB3	2.11	0.49
1:B:155:ILE:O	1:B:159:GLU:HB2	2.12	0.49
1:B:163:THR:CG2	1:B:202:GLU:HB2	2.43	0.49
1:D:170:LEU:O	1:D:174:PHE:HB2	2.11	0.49
1:C:27:LYS:HA	1:C:100:LEU:HD21	1.93	0.49
1:A:77:GLN:O	1:A:81:GLU:HG3	2.12	0.49
1:A:155:ILE:O	1:A:159:GLU:HB2	2.12	0.49
1:B:36:LEU:HB2	1:B:118:TYR:OH	2.13	0.49
1:B:70:GLU:CA	1:B:76:GLN:HE22	2.19	0.49
1:B:36:LEU:HD12	1:B:105:LEU:HD11	1.93	0.49
1:B:94:CYS:O	1:B:98:LEU:HB2	2.13	0.49
1:C:163:THR:HG21	1:C:202:GLU:HB2	1.94	0.49
1:D:48:TYR:O	1:D:52:VAL:HG12	2.12	0.49
1:D:124:ASP:O	1:D:127:ARG:HB3	2.12	0.49
1:A:5:GLU:O	1:A:9:LYS:HG3	2.12	0.49
1:C:182:LEU:O	1:C:184:SER:N	2.45	0.49
1:B:48:TYR:O	1:B:52:VAL:HG12	2.12	0.48
1:B:80:ARG:HB2	1:B:80:ARG:NH1	2.27	0.48
1:D:200:ILE:HG12	1:D:218:MET:HE1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LYS:HG2	1:B:78:MET:HE3	1.95	0.48
1:D:195:ALA:HA	3:D:2030:HOH:O	2.13	0.48
1:A:94:CYS:CB	1:A:129:LEU:HD13	2.44	0.48
1:A:170:LEU:O	1:A:174:PHE:HB2	2.13	0.48
1:A:206:LEU:O	1:A:207:SER:O	2.31	0.48
1:B:14:GLU:HB2	1:B:22:MET:SD	2.53	0.48
1:A:30:THR:CG2	1:A:105:LEU:HD13	2.40	0.48
1:A:101:LEU:HA	1:A:105:LEU:HB2	1.95	0.48
1:C:11:LYS:CG	1:C:43:LEU:HD21	2.43	0.48
1:C:19:TYR:HA	1:C:22:MET:HB3	1.96	0.48
1:B:70:GLU:C	1:B:70:GLU:OE1	2.53	0.48
1:B:89:GLU:O	1:B:93:ILE:HG12	2.13	0.48
1:B:113:GLU:HB3	1:B:160:MET:HE3	1.95	0.48
1:D:157:LYS:O	1:D:157:LYS:HG2	2.13	0.48
1:A:112:ALA:HA	1:A:115:LYS:CE	2.43	0.47
1:B:170:LEU:O	1:B:174:PHE:HB2	2.13	0.47
1:C:172:LEU:HD11	1:C:224:ASN:HD21	1.76	0.47
1:A:172:LEU:CD1	1:A:224:ASN:ND2	2.74	0.47
1:C:30:THR:CG2	1:C:100:LEU:HG	2.42	0.47
1:C:78:MET:SD	1:D:9:LYS:HG2	2.54	0.47
1:A:14:GLU:HB2	1:A:22:MET:SD	2.54	0.47
1:A:80:ARG:HB2	1:A:80:ARG:NH1	2.28	0.47
1:B:110:SER:O	1:B:115:LYS:HE2	2.15	0.47
1:C:101:LEU:HA	1:C:105:LEU:HB2	1.96	0.47
1:D:94:CYS:HB2	1:D:129:LEU:HD13	1.95	0.47
1:A:151:GLU:O	1:A:155:ILE:HG13	2.15	0.47
1:B:113:GLU:CB	1:B:160:MET:HE3	2.44	0.47
1:B:124:ASP:O	1:B:127:ARG:HB3	2.14	0.47
1:B:151:GLU:O	1:B:155:ILE:HG13	2.15	0.47
1:B:163:THR:HG21	1:B:202:GLU:HB2	1.96	0.47
1:C:36:LEU:HD12	1:C:105:LEU:HD11	1.96	0.47
1:D:36:LEU:HD12	1:D:105:LEU:HD11	1.96	0.47
1:D:101:LEU:HA	1:D:105:LEU:HB2	1.96	0.47
1:C:214:SER:O	1:C:218:MET:HG3	2.14	0.47
1:D:206:LEU:O	1:D:209:GLU:N	2.47	0.47
1:C:106:ILE:HD13	1:C:119:LEU:CD1	2.45	0.47
1:D:106:ILE:HD13	1:D:119:LEU:CD1	2.44	0.47
1:A:176:VAL:HG13	2:P:756:SER:HB2	1.97	0.47
1:B:49:LYS:HE3	3:B:2013:HOH:O	2.15	0.47
1:A:161:GLN:NE2	1:A:163:THR:OG1	2.48	0.46
1:C:173:ASN:OD1	2:R:758:TPO:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:PHE:O	1:D:181:ILE:HB	2.13	0.46
1:C:94:CYS:HB2	1:C:129:LEU:HD13	1.97	0.46
1:C:226:THR:HG22	1:C:227:LEU:HD12	1.97	0.46
1:A:72:ALA:HB3	1:A:75:LYS:CB	2.46	0.46
1:C:110:SER:O	1:C:115:LYS:HE2	2.16	0.46
1:A:90:LEU:HD23	1:A:90:LEU:C	2.36	0.46
1:A:116:VAL:HG21	1:A:156:SER:HB3	1.97	0.46
1:A:174:PHE:O	1:A:177:PHE:HB3	2.15	0.46
1:B:5:GLU:O	1:B:9:LYS:HG3	2.15	0.46
1:C:48:TYR:CD2	1:C:97:VAL:HG22	2.51	0.46
1:B:106:ILE:HD13	1:B:119:LEU:CD1	2.45	0.46
1:C:14:GLU:HB2	1:C:22:MET:SD	2.55	0.46
1:C:80:ARG:HB2	1:C:80:ARG:NH1	2.29	0.46
1:D:136:ASP:C	1:D:138:LYS:H	2.18	0.46
1:A:48:TYR:CD2	1:A:97:VAL:HG22	2.51	0.46
1:B:38:ASN:HB3	3:B:2010:HOH:O	2.16	0.46
1:B:192:ALA:HB2	1:B:228:TRP:HZ3	1.82	0.45
1:B:127:ARG:NH2	2:Q:758:TPO:HG21	2.31	0.45
1:D:111:GLN:HB2	1:D:114:SER:OG	2.15	0.45
1:B:226:THR:HG22	1:B:227:LEU:HD12	1.98	0.45
1:C:9:LYS:HG2	1:D:78:MET:SD	2.57	0.45
1:B:30:THR:HG23	1:B:105:LEU:HD13	1.97	0.45
1:B:94:CYS:HB2	1:B:129:LEU:HD13	1.98	0.45
1:D:226:THR:HG22	1:D:227:LEU:HD12	1.99	0.45
1:C:89:GLU:O	1:C:93:ILE:HG12	2.17	0.45
1:D:196:PHE:HE1	1:D:218:MET:HE2	1.82	0.45
1:B:136:ASP:C	1:B:138:LYS:N	2.70	0.45
1:B:203:LEU:O	1:B:206:LEU:HD11	2.17	0.45
1:C:136:ASP:C	1:C:138:LYS:N	2.70	0.45
1:A:110:SER:O	1:A:115:LYS:HE2	2.16	0.45
1:B:111:GLN:HB2	1:B:114:SER:OG	2.17	0.45
1:B:116:VAL:HG21	1:B:156:SER:HB3	1.98	0.45
1:C:111:GLN:HB2	1:C:114:SER:OG	2.17	0.45
1:A:218:MET:HA	1:A:221:LEU:HD12	1.99	0.45
1:D:116:VAL:HG21	1:D:156:SER:HB3	1.98	0.45
1:A:214:SER:O	1:A:218:MET:HG3	2.17	0.44
1:B:19:TYR:HA	1:B:22:MET:HB3	1.99	0.44
1:B:67:GLN:HA	1:B:70:GLU:HB2	2.00	0.44
1:C:9:LYS:HG2	1:D:78:MET:HE1	1.96	0.44
1:C:113:GLU:HB3	1:C:160:MET:HE3	1.99	0.44
1:C:151:GLU:O	1:C:155:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ASP:HA	1:C:216:LEU:HD12	1.99	0.44
1:D:5:GLU:O	1:D:9:LYS:HG3	2.16	0.44
1:C:31:GLU:HA	1:C:104:PHE:CE2	2.53	0.44
1:C:143:ASP:OD2	1:C:147:GLN:NE2	2.51	0.44
1:D:112:ALA:HA	1:D:115:LYS:CE	2.47	0.44
1:C:116:VAL:HG21	1:C:156:SER:HB3	2.00	0.44
1:C:193:LYS:HG3	1:C:225:LEU:HD22	1.98	0.44
1:A:193:LYS:O	1:A:196:PHE:N	2.49	0.44
1:C:91:ARG:HG3	1:C:129:LEU:HD11	1.99	0.44
1:C:124:ASP:O	1:C:127:ARG:HB3	2.17	0.44
1:C:160:MET:HE2	1:C:164:HIS:CD2	2.53	0.44
1:D:110:SER:O	1:D:115:LYS:HE2	2.18	0.44
1:D:164:HIS:CD2	1:D:166:ILE:HB	2.52	0.44
1:A:136:ASP:C	1:A:138:LYS:N	2.71	0.44
1:C:164:HIS:CD2	1:C:166:ILE:HB	2.53	0.44
1:D:151:GLU:O	1:D:155:ILE:HG13	2.18	0.44
2:P:759:THR:CG2	2:P:760:THR:N	2.81	0.44
1:A:106:ILE:HD13	1:A:119:LEU:CD1	2.47	0.44
2:S:757:ALA:O	2:S:758:TPO:HG22	2.17	0.44
1:C:136:ASP:C	1:C:138:LYS:H	2.20	0.43
1:C:184:SER:OG	1:C:187:LYS:HG3	2.17	0.43
1:A:78:MET:SD	1:B:9:LYS:HG2	2.58	0.43
1:A:177:PHE:O	1:A:181:ILE:HB	2.19	0.43
1:B:203:LEU:O	1:B:206:LEU:HG	2.18	0.43
1:D:119:LEU:HB3	1:D:152:ALA:HB2	2.00	0.43
1:D:136:ASP:C	1:D:138:LYS:N	2.69	0.43
1:B:214:SER:O	1:B:218:MET:HG3	2.17	0.43
1:C:10:ALA:O	1:C:22:MET:HG3	2.18	0.43
1:B:67:GLN:O	1:B:70:GLU:N	2.50	0.43
1:B:84:GLU:O	1:B:88:THR:HG23	2.19	0.43
1:B:136:ASP:C	1:B:138:LYS:H	2.21	0.43
1:B:187:LYS:O	1:B:190:SER:HB2	2.19	0.43
1:C:163:THR:HB	1:C:206:LEU:HD21	2.00	0.43
1:C:187:LYS:O	1:C:190:SER:HB2	2.19	0.43
1:D:83:ARG:O	1:D:87:GLU:HB2	2.18	0.43
1:D:187:LYS:O	1:D:190:SER:HB2	2.19	0.43
1:C:192:ALA:HB3	1:C:225:LEU:CD2	2.39	0.43
1:A:90:LEU:HD23	1:A:90:LEU:O	2.19	0.43
1:A:19:TYR:HA	1:A:22:MET:HB3	2.01	0.43
1:B:85:LYS:CE	3:B:2018:HOH:O	2.67	0.43
1:B:127:ARG:HH22	2:Q:758:TPO:P	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:MET:HE2	1:D:12:LEU:HD23	2.01	0.43
1:B:220:LEU:HA	1:B:220:LEU:HD23	1.83	0.43
1:D:168:LEU:HB3	1:D:217:ILE:HG21	2.01	0.43
1:B:10:ALA:O	1:B:22:MET:HG3	2.18	0.42
2:Q:759:THR:CG2	2:Q:760:THR:N	2.82	0.42
1:C:218:MET:HA	1:C:221:LEU:HD12	2.01	0.42
1:B:41:ARG:HG3	1:B:118:TYR:CZ	2.53	0.42
1:B:91:ARG:HG3	1:B:129:LEU:HD11	2.01	0.42
1:D:11:LYS:CG	1:D:43:LEU:HD21	2.49	0.42
1:A:41:ARG:NH1	1:A:113:GLU:OE2	2.43	0.42
1:A:56:ARG:NH1	1:A:128:TYR:CE1	2.87	0.42
1:A:161:GLN:NE2	1:A:163:THR:CG2	2.82	0.42
1:A:83:ARG:O	1:A:87:GLU:HB2	2.20	0.42
1:A:120:LYS:NZ	3:A:2030:HOH:O	2.41	0.42
1:A:136:ASP:C	1:A:138:LYS:H	2.23	0.42
1:D:120:LYS:HE2	1:D:173:ASN:OD1	2.19	0.42
1:B:11:LYS:CG	1:B:43:LEU:HD21	2.49	0.42
1:B:192:ALA:HB3	1:B:225:LEU:HD21	2.00	0.42
1:D:119:LEU:HD12	1:D:119:LEU:HA	1.89	0.42
1:D:196:PHE:CE1	1:D:218:MET:HE2	2.54	0.42
1:A:179:TYR:CZ	1:A:228:TRP:CD1	3.08	0.42
1:B:177:PHE:O	1:B:181:ILE:HB	2.19	0.42
1:C:119:LEU:HB3	1:C:152:ALA:HB2	2.01	0.42
1:A:10:ALA:O	1:A:22:MET:HG3	2.20	0.42
2:S:759:THR:CG2	2:S:760:THR:N	2.82	0.42
1:A:187:LYS:O	1:A:190:SER:HB2	2.20	0.42
1:A:196:PHE:CE2	1:A:200:ILE:HD11	2.55	0.42
1:D:187:LYS:HA	1:D:190:SER:OG	2.19	0.42
1:A:16:ALA:HB2	1:B:62:VAL:CG2	2.50	0.42
1:B:119:LEU:HB3	1:B:152:ALA:HB2	2.02	0.42
1:B:143:ASP:OD2	1:B:147:GLN:NE2	2.53	0.42
1:B:213:ASP:HA	1:B:216:LEU:HD12	2.02	0.42
1:C:177:PHE:O	1:C:181:ILE:HB	2.19	0.42
1:C:187:LYS:HA	1:C:190:SER:OG	2.20	0.42
1:D:214:SER:O	1:D:218:MET:HG3	2.20	0.42
1:B:94:CYS:CB	1:B:129:LEU:HD13	2.50	0.41
1:B:168:LEU:HD21	1:B:199:ALA:HB2	2.02	0.41
1:D:36:LEU:HD11	1:D:105:LEU:HD11	2.02	0.41
1:A:91:ARG:HG3	1:A:129:LEU:HD11	2.03	0.41
1:B:126:TYR:CE1	1:C:0:SER:HB3	2.55	0.41
1:C:35:GLU:HG2	3:C:2028:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:GLU:O	1:C:9:LYS:HG3	2.19	0.41
1:C:36:LEU:HB2	1:C:118:TYR:OH	2.19	0.41
1:D:27:LYS:HE3	3:D:2008:HOH:O	2.20	0.41
1:D:218:MET:HA	1:D:221:LEU:HB2	2.02	0.41
1:C:83:ARG:O	1:C:87:GLU:HB2	2.20	0.41
1:C:218:MET:HA	1:C:221:LEU:HB2	2.02	0.41
1:A:206:LEU:HD22	1:A:214:SER:CB	2.51	0.41
1:C:90:LEU:HD23	1:C:90:LEU:O	2.21	0.41
1:C:120:LYS:NZ	3:C:2030:HOH:O	2.48	0.41
1:C:90:LEU:HD23	1:C:90:LEU:C	2.40	0.41
1:A:89:GLU:O	1:A:93:ILE:HG12	2.21	0.41
1:C:150:GLN:NE2	1:C:154:GLU:HG3	2.33	0.41
1:C:193:LYS:HG3	1:C:225:LEU:CD2	2.51	0.41
1:C:205:THR:O	1:C:206:LEU:C	2.59	0.41
1:D:89:GLU:O	1:D:93:ILE:HG12	2.20	0.41
1:C:48:TYR:CG	1:C:97:VAL:HG22	2.55	0.41
1:C:100:LEU:HD12	1:C:100:LEU:HA	1.97	0.41
1:D:84:GLU:O	1:D:88:THR:HG23	2.21	0.41
1:A:119:LEU:HB3	1:A:152:ALA:HB2	2.03	0.41
1:A:163:THR:HB	1:A:206:LEU:HD21	2.03	0.41
1:B:172:LEU:CD1	1:B:224:ASN:ND2	2.84	0.41
1:C:84:GLU:O	1:C:88:THR:HG23	2.21	0.41
1:C:172:LEU:CD1	1:C:224:ASN:HD22	2.34	0.41
1:D:19:TYR:HA	1:D:22:MET:HB3	2.02	0.41
1:D:60:ARG:HD3	3:D:2012:HOH:O	2.20	0.41
1:D:94:CYS:CB	1:D:129:LEU:HD13	2.50	0.41
1:D:136:ASP:O	1:D:138:LYS:N	2.54	0.41
1:D:205:THR:O	1:D:206:LEU:C	2.58	0.41
1:A:84:GLU:O	1:A:88:THR:HG23	2.21	0.41
1:D:91:ARG:HG3	1:D:129:LEU:HD11	2.03	0.41
1:A:220:LEU:HD23	1:A:220:LEU:HA	1.88	0.40
1:B:153:PHE:N	1:B:170:LEU:HD21	2.37	0.40
1:B:112:ALA:HA	1:B:115:LYS:CE	2.45	0.40
1:B:150:GLN:NE2	1:B:154:GLU:HG3	2.32	0.40
1:C:11:LYS:HD3	1:C:43:LEU:HD21	2.03	0.40
1:C:113:GLU:CB	1:C:160:MET:HE3	2.51	0.40
1:C:168:LEU:HD21	1:C:199:ALA:HB2	2.04	0.40
1:D:218:MET:HA	1:D:221:LEU:HD12	2.03	0.40
1:A:31:GLU:HA	1:A:104:PHE:CE2	2.56	0.40
1:A:122:LYS:HD2	3:A:2032:HOH:O	2.20	0.40
1:D:90:LEU:C	1:D:90:LEU:HD23	2.41	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	225/247 (91%)	192 (85%)	27 (12%)	6 (3%)	5 7
1	B	221/247 (90%)	191 (86%)	26 (12%)	4 (2%)	8 14
1	C	221/247 (90%)	187 (85%)	28 (13%)	6 (3%)	5 7
1	D	222/247 (90%)	187 (84%)	31 (14%)	4 (2%)	8 14
2	P	5/10 (50%)	2 (40%)	2 (40%)	1 (20%)	0 0
2	Q	5/10 (50%)	2 (40%)	2 (40%)	1 (20%)	0 0
2	R	5/10 (50%)	2 (40%)	2 (40%)	1 (20%)	0 0
2	S	5/10 (50%)	2 (40%)	2 (40%)	1 (20%)	0 0
All	All	909/1028 (88%)	765 (84%)	120 (13%)	24 (3%)	5 8

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	ASN
1	A	208	GLU
1	A	211	TYR
1	B	183	ASN
1	B	211	TYR
1	C	68	LYS
1	C	183	ASN
1	C	211	TYR
1	D	183	ASN
1	D	211	TYR
1	A	206	LEU
1	A	207	SER
1	A	212	LYS
1	B	212	LYS

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Mol	Chain	Res	Type
1	C	212	LYS
1	D	212	LYS
2	Q	759	THR
2	S	759	THR
2	R	759	THR
1	C	138	LYS
2	P	759	THR
1	B	138	LYS
1	C	139	LYS
1	D	138	LYS

5.3.2 Protein sidechains (i)

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	198/210 (94%)	181 (91%)	17 (9%)	10	20
1	B	197/210 (94%)	177 (90%)	20 (10%)	7	14
1	C	197/210 (94%)	179 (91%)	18 (9%)	9	18
1	D	197/210 (94%)	178 (90%)	19 (10%)	8	16
2	P	5/8 (62%)	5 (100%)	0	100	100
2	Q	5/8 (62%)	5 (100%)	0	100	100
2	R	5/8 (62%)	5 (100%)	0	100	100
2	S	5/8 (62%)	5 (100%)	0	100	100
All	All	809/872 (93%)	735 (91%)	74 (9%)	9	18

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASP
1	A	26	MET
1	A	43	LEU
1	A	50	ASN
1	A	77	GLN

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Mol	Chain	Res	Type
1	A	78	MET
1	A	80	ARG
1	A	98	LEU
1	A	105	LEU
1	A	113	GLU
1	A	124	ASP
1	A	126	TYR
1	A	137	ASP
1	A	163	THR
1	A	174	PHE
1	A	183	ASN
1	A	219	GLN
1	B	20	ASP
1	B	26	MET
1	B	43	LEU
1	B	50	ASN
1	B	70	GLU
1	B	77	GLN
1	B	78	MET
1	B	80	ARG
1	B	98	LEU
1	B	105	LEU
1	B	113	GLU
1	B	124	ASP
1	B	126	TYR
1	B	137	ASP
1	B	144	GLN
1	B	163	THR
1	B	174	PHE
1	B	183	ASN
1	B	206	LEU
1	B	219	GLN
1	C	20	ASP
1	C	26	MET
1	C	43	LEU
1	C	50	ASN
1	C	77	GLN
1	C	78	MET
1	C	80	ARG
1	C	98	LEU
1	C	105	LEU
1	C	113	GLU

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Mol	Chain	Res	Type
1	C	124	ASP
1	C	126	TYR
1	C	137	ASP
1	C	144	GLN
1	C	163	THR
1	C	174	PHE
1	C	183	ASN
1	C	219	GLN
1	D	20	ASP
1	D	26	MET
1	D	43	LEU
1	D	50	ASN
1	D	77	GLN
1	D	78	MET
1	D	80	ARG
1	D	98	LEU
1	D	105	LEU
1	D	113	GLU
1	D	124	ASP
1	D	126	TYR
1	D	137	ASP
1	D	144	GLN
1	D	163	THR
1	D	174	PHE
1	D	183	ASN
1	D	189	CYS
1	D	219	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	15	GLN
1	A	77	GLN
1	A	95	ASN
1	A	144	GLN
1	A	146	GLN
1	A	150	GLN
1	A	161	GLN
1	A	183	ASN
1	B	8	GLN
1	B	15	GLN

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Mol	Chain	Res	Type
1	B	42	ASN
1	B	76	GLN
1	B	77	GLN
1	B	150	GLN
1	B	164	HIS
1	B	183	ASN
1	B	224	ASN
1	C	8	GLN
1	C	15	GLN
1	C	77	GLN
1	C	95	ASN
1	C	150	GLN
1	C	164	HIS
1	C	183	ASN
1	C	224	ASN
1	D	8	GLN
1	D	15	GLN
1	D	77	GLN
1	D	95	ASN
1	D	146	GLN
1	D	150	GLN
1	D	173	ASN
1	D	183	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	TPO	S	758	2	8,10,11	1.06	0	10,14,16	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TPO	P	758	2	8,10,11	1.06	0	10,14,16	0.82	0
2	TPO	R	758	2	8,10,11	1.04	0	10,14,16	0.90	0
2	TPO	Q	758	2	8,10,11	1.07	0	10,14,16	0.89	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	TPO	S	758	2	-	3/9/11/13	-
2	TPO	P	758	2	-	3/9/11/13	-
2	TPO	R	758	2	-	3/9/11/13	-
2	TPO	Q	758	2	-	2/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	758	TPO	CB-OG1-P-O1P
2	Q	758	TPO	CB-OG1-P-O1P
2	R	758	TPO	CB-OG1-P-O1P
2	S	758	TPO	CB-OG1-P-O1P
2	P	758	TPO	CB-OG1-P-O3P
2	R	758	TPO	CB-OG1-P-O3P
2	S	758	TPO	CB-OG1-P-O3P
2	P	758	TPO	O-C-CA-CB
2	Q	758	TPO	O-C-CA-CB
2	R	758	TPO	O-C-CA-CB
2	S	758	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	758	TPO	3	0
2	P	758	TPO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	758	TPO	5	0
2	Q	758	TPO	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	229/247 (92%)	0.75	19 (8%)	11	11	24, 64, 82, 93	0
1	B	227/247 (91%)	0.89	24 (10%)	6	5	34, 69, 91, 98	0
1	C	227/247 (91%)	0.83	26 (11%)	4	4	20, 70, 88, 95	0
1	D	228/247 (92%)	0.84	22 (9%)	8	7	11, 65, 84, 90	0
2	P	7/10 (70%)	0.13	0	100	100	58, 63, 71, 75	0
2	Q	7/10 (70%)	0.68	0	100	100	64, 68, 71, 73	0
2	R	7/10 (70%)	1.31	2 (28%)	0	0	65, 70, 84, 86	0
2	S	7/10 (70%)	1.30	1 (14%)	2	2	63, 66, 73, 76	0
All	All	939/1028 (91%)	0.83	94 (10%)	7	6	11, 67, 87, 98	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	69	THR	5.9
2	S	762	MET	5.8
1	D	211	TYR	5.6
1	B	211	TYR	5.2
1	D	227	LEU	4.9
1	A	227	LEU	4.8
1	B	227	LEU	4.8
1	B	69	THR	4.4
1	B	222	ARG	4.3
1	B	195	ALA	4.2
1	D	34	ALA	4.1
1	C	206	LEU	4.0
1	B	75	LYS	4.0
1	D	134	ALA	4.0
1	D	230	SER	3.9
2	R	755	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	205	THR	3.9
1	A	77	GLN	3.8
1	B	74	LYS	3.7
1	D	229	THR	3.7
1	D	111	GLN	3.7
1	D	191	LEU	3.7
1	D	202	GLU	3.5
1	B	191	LEU	3.4
1	C	227	LEU	3.3
1	B	135	GLY	3.2
1	C	134	ALA	3.2
1	C	69	THR	3.2
1	C	75	LYS	3.2
1	A	186	GLU	3.1
1	A	203	LEU	3.1
1	B	157	LYS	3.1
1	D	203	LEU	3.0
1	A	229	THR	3.0
1	B	205	THR	3.0
1	B	-1	GLY	3.0
1	C	212	LYS	3.0
1	D	206	LEU	3.0
1	C	225	LEU	2.9
1	A	206	LEU	2.9
1	B	206	LEU	2.9
1	D	185	PRO	2.9
1	B	204	ASP	2.8
1	D	68	LYS	2.8
1	C	208	GLU	2.8
1	D	153	PHE	2.7
1	D	157	LYS	2.7
1	A	230	SER	2.7
1	C	203	LEU	2.7
1	D	210	SER	2.6
1	C	216	LEU	2.6
1	C	-1	GLY	2.5
1	C	191	LEU	2.5
1	B	216	LEU	2.5
1	C	195	ALA	2.5
2	R	759	THR	2.5
1	B	209	GLU	2.5
1	D	205	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	153	PHE	2.4
1	C	78	MET	2.4
1	B	115	LYS	2.4
1	C	73	GLU	2.4
1	B	183	ASN	2.4
1	D	224	ASN	2.4
1	A	226	THR	2.3
1	C	161	GLN	2.3
1	B	109	ALA	2.3
1	C	179	TYR	2.3
1	A	63	SER	2.3
1	D	228	TRP	2.3
1	B	187	LYS	2.3
1	C	80	ARG	2.2
1	C	0	SER	2.2
1	C	185	PRO	2.2
1	A	183	ASN	2.2
1	D	161	GLN	2.2
1	A	161	GLN	2.2
1	A	208	GLU	2.2
1	A	72	ALA	2.2
1	B	161	GLN	2.1
1	A	74	LYS	2.1
1	C	228	TRP	2.1
1	A	67	GLN	2.1
1	C	77	GLN	2.1
1	B	179	TYR	2.1
1	A	111	GLN	2.1
1	A	211	TYR	2.0
1	C	159	GLU	2.0
1	A	65	ILE	2.0
1	B	153	PHE	2.0
1	C	160	MET	2.0
1	A	115	LYS	2.0
1	B	0	SER	2.0
1	D	213	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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(Å^2)	Q<0.9
2	TPO	P	758	11/12	0.92	0.14	45,50,58,58	0
2	TPO	S	758	11/12	0.93	0.15	47,54,63,64	0
2	TPO	Q	758	11/12	0.95	0.15	63,65,66,66	0
2	TPO	R	758	11/12	0.96	0.15	50,56,67,70	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.