Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 04:32 AM EDT

PDB ID	:	4I5O
Title	:	Crystal Structure of W-W-R ClpX Hexamer
Authors	:	Glynn, S.E.; Nager, A.R.; Stinson, B.S.; Schmitz, K.R.; Baker, T.A.; Sauer, R.T.
Deposited on	:	2012-11-28
Resolution	:	4.48 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:

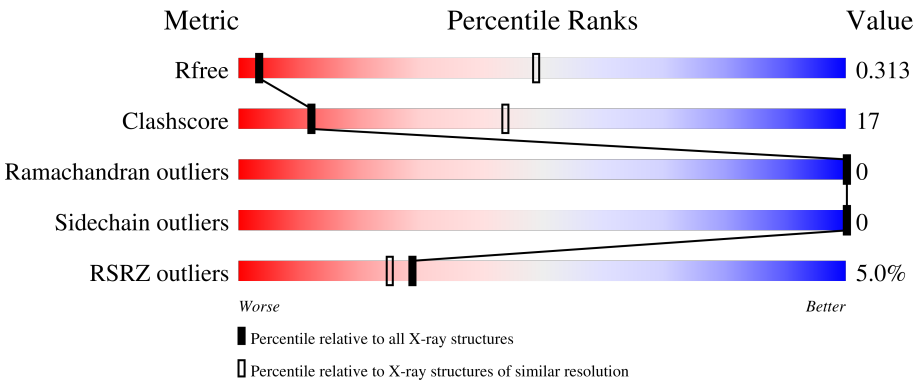
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 4.48 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	1051 (5.12-3.80)
Clashscore	141614	1119 (5.12-3.80)
Ramachandran outliers	138981	1065 (5.12-3.80)
Sidechain outliers	138945	1047 (5.12-3.80)
RSRZ outliers	127900	1099 (5.20-3.70)

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 <=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	363	5% 58% 27% 15%
1	B	363	3% 53% 31% 15%
1	C	363	7% 58% 29% 13%
1	D	363	4% 57% 27% 16%
1	E	363	4% 59% 29% 12%

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Mol	Chain	Length	Quality of chain
1	F	363	4% 56% 29% 15%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	501	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13980 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.

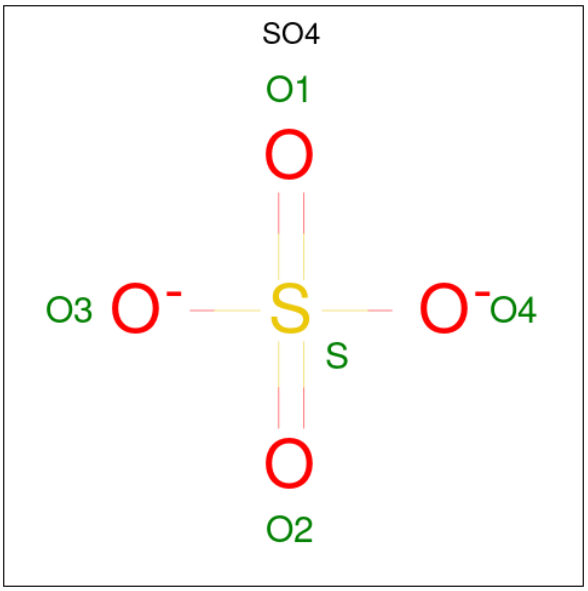
- Molecule 1 is a protein called ATP-dependent Clp protease ATP-binding subunit ClpX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	309	2317	1475	384	452	6	0	0	0
1	B	308	2312	1472	383	451	6	0	0	0
1	C	317	2342	1488	388	462	4	0	0	0
1	D	304	2294	1462	377	449	6	0	0	0
1	E	318	2365	1505	393	461	6	0	0	0
1	F	310	2320	1479	383	452	6	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	GLU	LYS	conflict	UNP P0A6H1
B	408	GLU	LYS	conflict	UNP P0A6H1
C	408	GLU	LYS	conflict	UNP P0A6H1
D	408	GLU	LYS	conflict	UNP P0A6H1
E	408	GLU	LYS	conflict	UNP P0A6H1
F	408	GLU	LYS	conflict	UNP P0A6H1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



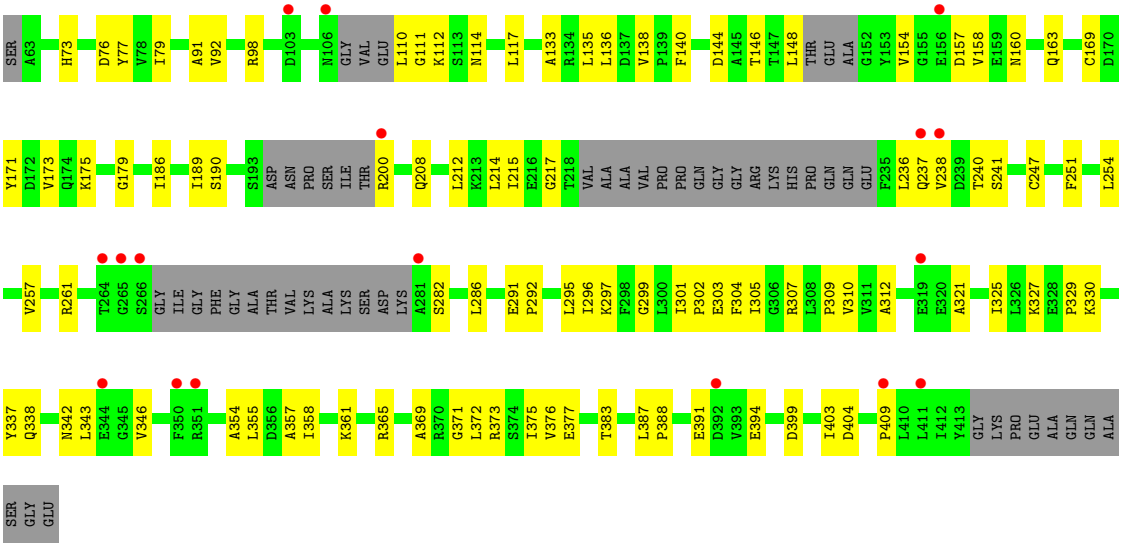
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	F	1	5	4	1	0	0

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.

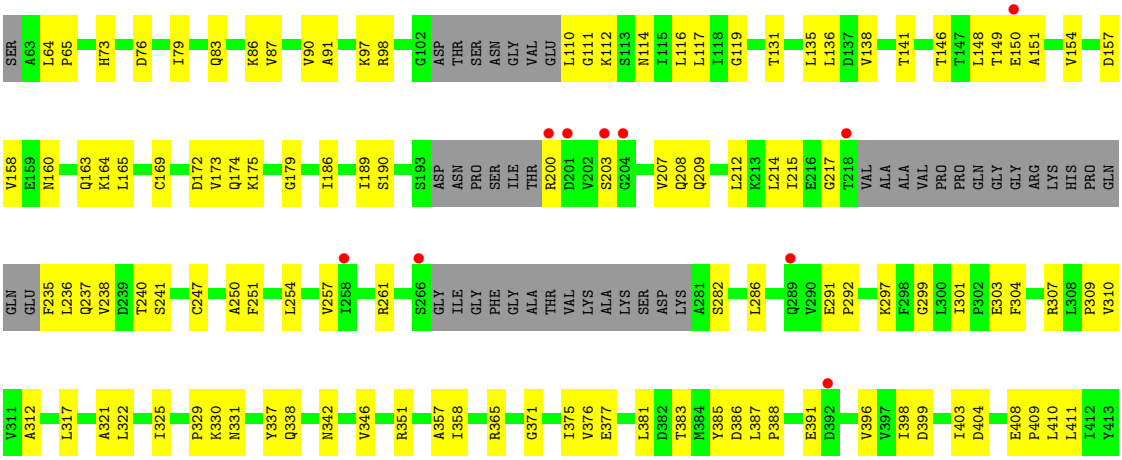
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain A:



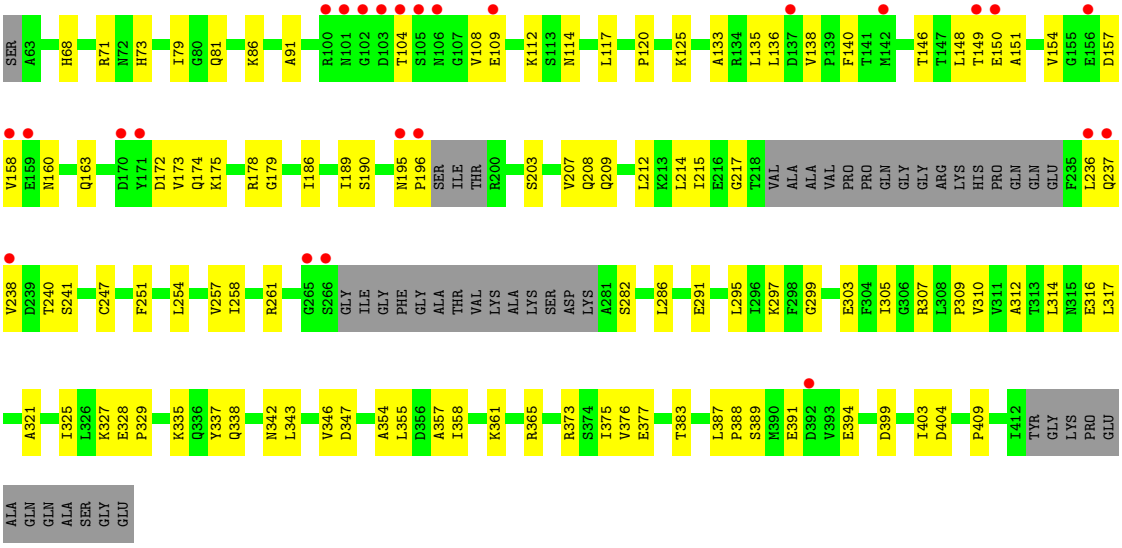
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain B:



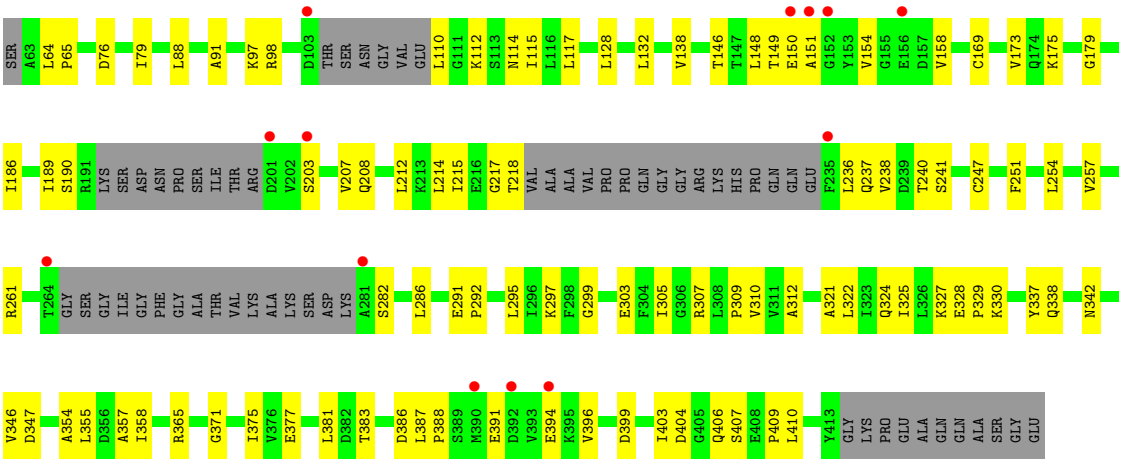
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain C:



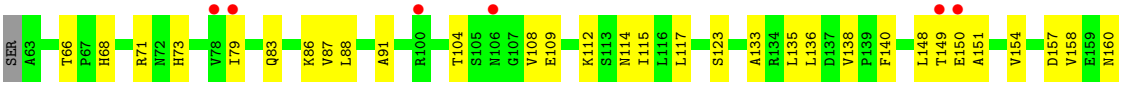
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

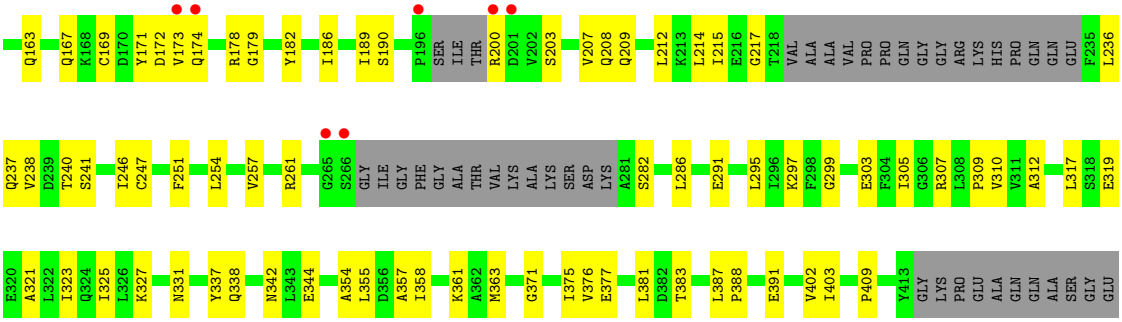
Chain D:



• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

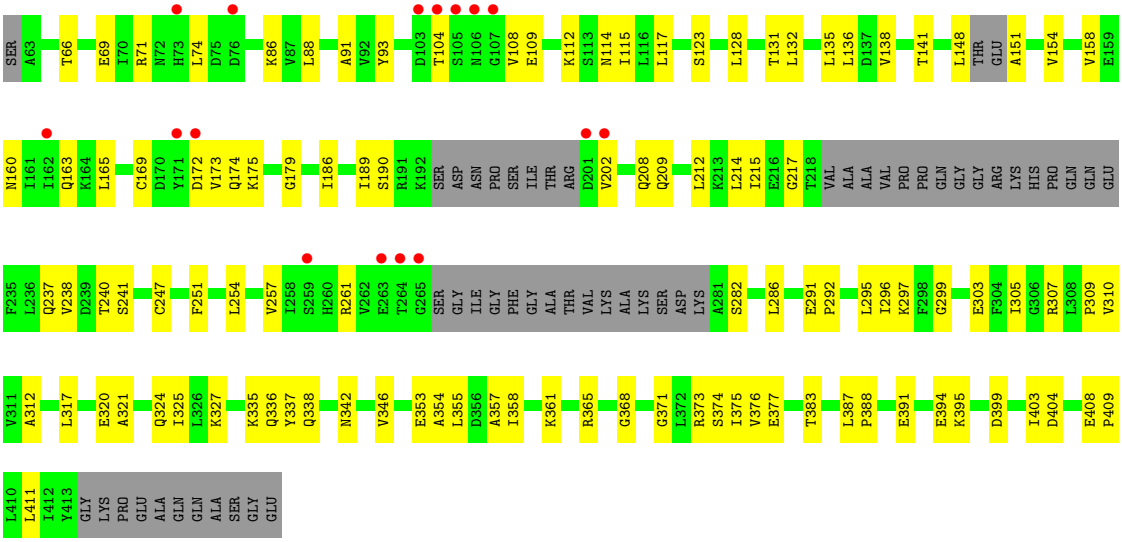
Chain E:





- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.20Å 199.88Å 222.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.32 – 4.48 48.32 – 4.48	Depositor EDS
% Data completeness (in resolution range)	91.5 (48.32-4.48) 91.5 (48.32-4.48)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.26 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.286 , 0.323 0.286 , 0.313	Depositor DCC
R_{free} test set	714 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	163.5	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 186.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	13980	wwPDB-VP
Average B, all atoms (Å^2)	222.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: 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	0.21	0/2341	0.36	0/3168
1	B	0.21	0/2337	0.38	0/3164
1	C	0.21	0/2368	0.38	0/3215
1	D	0.21	0/2319	0.38	0/3140
1	E	0.21	0/2392	0.38	0/3243
1	F	0.21	0/2345	0.37	0/3175
All	All	0.21	0/14102	0.37	0/19105

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	2317	0	2312	81	0
1	B	2312	0	2314	91	0
1	C	2342	0	2310	90	0
1	D	2294	0	2301	79	0
1	E	2365	0	2348	85	0
1	F	2320	0	2323	88	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
All	All	13980	0	13908	479	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 (479) 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:C:150:GLU:HA	1:C:203:SER:HB2	1.42	1.00
1:B:215:ILE:HG21	1:B:307:ARG:HB3	1.45	0.97
1:D:215:ILE:HG21	1:D:307:ARG:HB3	1.49	0.94
1:A:215:ILE:HG21	1:A:307:ARG:HB3	1.49	0.94
1:F:215:ILE:HG21	1:F:307:ARG:HB3	1.50	0.94
1:E:215:ILE:HG21	1:E:307:ARG:HB3	1.52	0.92
1:C:215:ILE:HG21	1:C:307:ARG:HB3	1.51	0.91
1:E:150:GLU:HA	1:E:203:SER:HB2	1.52	0.90
1:D:150:GLU:HA	1:D:203:SER:HB2	1.54	0.89
1:C:186:ILE:HG13	1:C:247:CYS:HB3	1.53	0.87
1:B:150:GLU:HA	1:B:203:SER:HB2	1.58	0.84
1:E:186:ILE:HG13	1:E:247:CYS:HB3	1.61	0.83
1:B:76:ASP:HB3	1:B:330:LYS:HE3	1.61	0.82
1:B:112:LYS:HE3	1:B:307:ARG:HE	1.44	0.82
1:B:186:ILE:HG13	1:B:247:CYS:HB3	1.61	0.81
1:C:112:LYS:HE3	1:C:307:ARG:HE	1.43	0.81
1:A:112:LYS:HE3	1:A:307:ARG:HE	1.45	0.81
1:E:112:LYS:HE3	1:E:307:ARG:HE	1.44	0.80
1:F:112:LYS:HE3	1:F:307:ARG:HE	1.47	0.80
1:D:381:LEU:HD11	1:E:86:LYS:HD2	1.64	0.79
1:C:173:VAL:HG13	1:C:238:VAL:HG22	1.64	0.78
1:D:148:LEU:HA	1:D:154:VAL:HG21	1.66	0.78
1:B:79:ILE:HD11	1:B:329:PRO:HD3	1.66	0.78
1:D:76:ASP:HB3	1:D:330:LYS:HE3	1.64	0.78
1:E:104:THR:OG1	1:E:108:VAL:HB	1.84	0.77
1:F:186:ILE:HG13	1:F:247:CYS:HB3	1.66	0.77
1:F:337:TYR:OH	1:F:377:GLU:HG2	1.84	0.77
1:D:79:ILE:HD11	1:D:329:PRO:HD3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:TYR:OH	1:B:377:GLU:HG2	1.84	0.77
1:A:173:VAL:HG13	1:A:238:VAL:HG22	1.68	0.76
1:B:114:ASN:ND2	1:B:215:ILE:HG23	2.00	0.76
1:C:357:ALA:HB1	1:C:403:ILE:HG23	1.68	0.76
1:A:76:ASP:HB3	1:A:330:LYS:HE3	1.68	0.75
1:D:112:LYS:HE3	1:D:307:ARG:HE	1.51	0.75
1:F:357:ALA:HB1	1:F:403:ILE:HG23	1.67	0.75
1:A:337:TYR:OH	1:A:377:GLU:HG2	1.87	0.74
1:A:357:ALA:HB1	1:A:403:ILE:HG23	1.68	0.74
1:A:79:ILE:HD11	1:A:329:PRO:HD3	1.70	0.74
1:B:357:ALA:HB1	1:B:403:ILE:HG23	1.69	0.74
1:B:173:VAL:HG13	1:B:238:VAL:HG22	1.69	0.73
1:D:337:TYR:OH	1:D:377:GLU:HG2	1.88	0.73
1:B:148:LEU:HA	1:B:154:VAL:HG21	1.70	0.73
1:A:214:LEU:HD22	1:A:240:THR:HG21	1.69	0.72
1:C:214:LEU:HD22	1:C:240:THR:HG21	1.71	0.72
1:A:148:LEU:HA	1:A:154:VAL:HG21	1.71	0.72
1:E:71:ARG:HH12	1:E:86:LYS:HE2	1.55	0.71
1:B:214:LEU:HD22	1:B:240:THR:HG21	1.73	0.71
1:D:186:ILE:HG13	1:D:247:CYS:HB3	1.71	0.71
1:D:357:ALA:HB1	1:D:403:ILE:HG23	1.71	0.71
1:D:114:ASN:ND2	1:D:215:ILE:HG23	2.05	0.70
1:E:214:LEU:HD22	1:E:240:THR:HG21	1.73	0.70
1:A:114:ASN:ND2	1:A:215:ILE:HG23	2.06	0.70
1:B:387:LEU:HB3	1:B:388:PRO:HD3	1.71	0.70
1:F:148:LEU:HA	1:F:154:VAL:HG21	1.72	0.70
1:A:186:ILE:HG13	1:A:247:CYS:HB3	1.72	0.70
1:E:148:LEU:HA	1:E:154:VAL:HG21	1.72	0.70
1:E:357:ALA:HB1	1:E:403:ILE:HG23	1.73	0.70
1:A:111:GLY:HA2	1:F:373:ARG:NH1	2.06	0.70
1:C:327:LYS:HD2	1:C:355:LEU:HD13	1.73	0.69
1:E:387:LEU:HB3	1:E:388:PRO:HD3	1.72	0.69
1:F:403:ILE:HG13	1:F:404:ASP:H	1.58	0.69
1:C:114:ASN:ND2	1:C:215:ILE:HG23	2.09	0.68
1:F:214:LEU:HD22	1:F:240:THR:HG21	1.73	0.68
1:E:337:TYR:OH	1:E:377:GLU:HG2	1.93	0.68
1:C:148:LEU:HA	1:C:154:VAL:HG21	1.74	0.68
1:A:112:LYS:HZ3	1:F:373:ARG:HE	1.41	0.67
1:C:403:ILE:HG13	1:C:404:ASP:H	1.59	0.67
1:B:351:ARG:HD2	1:B:398:ILE:HG22	1.75	0.67
1:C:337:TYR:OH	1:C:377:GLU:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:THR:CB	1:E:108:VAL:HB	2.24	0.67
1:E:114:ASN:ND2	1:E:215:ILE:HG23	2.10	0.67
1:F:173:VAL:HG13	1:F:238:VAL:HG22	1.77	0.67
1:D:386:ASP:HB3	1:E:68:HIS:NE2	2.10	0.66
1:D:214:LEU:HD22	1:D:240:THR:HG21	1.77	0.66
1:D:387:LEU:HB3	1:D:388:PRO:HD3	1.76	0.66
1:F:114:ASN:ND2	1:F:215:ILE:HG23	2.10	0.66
1:C:151:ALA:HB3	1:C:154:VAL:HB	1.78	0.65
1:D:322:LEU:HD23	1:D:325:ILE:HD12	1.79	0.65
1:A:343:LEU:HD13	1:B:97:LYS:HE3	1.80	0.64
1:B:403:ILE:HG13	1:B:404:ASP:H	1.63	0.64
1:E:208:GLN:O	1:E:212:LEU:HB2	1.98	0.64
1:A:169:CYS:SG	1:A:175:LYS:HB2	2.38	0.63
1:A:387:LEU:HB3	1:A:388:PRO:HD3	1.80	0.63
1:C:387:LEU:HB3	1:C:388:PRO:HD3	1.80	0.63
1:A:338:GLN:O	1:A:342:ASN:HB2	1.99	0.63
1:B:381:LEU:HD11	1:C:86:LYS:HD2	1.82	0.62
1:D:403:ILE:HG13	1:D:404:ASP:H	1.64	0.62
1:D:321:ALA:O	1:D:325:ILE:HG13	2.00	0.62
1:C:79:ILE:HD12	1:C:321:ALA:HA	1.80	0.62
1:A:399:ASP:O	1:A:403:ILE:HG12	1.99	0.62
1:F:338:GLN:O	1:F:342:ASN:HB2	1.99	0.62
1:A:217:GLY:HA2	1:A:240:THR:OG1	2.01	0.61
1:B:321:ALA:O	1:B:325:ILE:HG13	2.01	0.61
1:D:151:ALA:HB3	1:D:154:VAL:HB	1.82	0.61
1:F:131:THR:O	1:F:135:LEU:HG	2.00	0.61
1:A:212:LEU:HD11	1:A:307:ARG:HG3	1.81	0.61
1:A:112:LYS:NZ	1:F:373:ARG:HE	1.98	0.61
1:A:403:ILE:HG13	1:A:404:ASP:H	1.66	0.61
1:A:208:GLN:O	1:A:212:LEU:HB2	2.00	0.61
1:B:383:THR:OG1	1:B:409:PRO:HG3	2.01	0.60
1:D:208:GLN:O	1:D:212:LEU:HB2	2.02	0.60
1:C:391:GLU:O	1:C:391:GLU:HG2	2.02	0.60
1:E:338:GLN:O	1:E:342:ASN:HB2	2.01	0.60
1:F:387:LEU:HB3	1:F:388:PRO:HD3	1.83	0.60
1:A:365:ARG:NH2	1:B:292:PRO:HG2	2.17	0.59
1:A:292:PRO:HG2	1:F:365:ARG:NH2	2.17	0.59
1:F:399:ASP:O	1:F:403:ILE:HG12	2.02	0.59
1:D:327:LYS:HD2	1:D:355:LEU:HD13	1.85	0.59
1:F:212:LEU:HD11	1:F:307:ARG:HG3	1.84	0.59
1:D:117:LEU:HD23	1:D:312:ALA:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:ALA:HB3	1:E:154:VAL:HB	1.84	0.59
1:B:114:ASN:HD22	1:B:215:ILE:HG23	1.66	0.59
1:B:399:ASP:O	1:B:403:ILE:HG12	2.02	0.59
1:B:151:ALA:HB3	1:B:154:VAL:HB	1.83	0.59
1:E:212:LEU:HD11	1:E:307:ARG:HG3	1.85	0.58
1:B:208:GLN:O	1:B:212:LEU:HB2	2.03	0.58
1:C:146:THR:HG22	1:D:218:THR:HA	1.85	0.58
1:F:208:GLN:O	1:F:212:LEU:HB2	2.03	0.58
1:B:117:LEU:HD23	1:B:312:ALA:HB3	1.84	0.58
1:B:154:VAL:O	1:B:158:VAL:HG23	2.03	0.58
1:F:395:LYS:HG2	1:F:411:LEU:HD22	1.86	0.58
1:D:173:VAL:HG13	1:D:238:VAL:HG22	1.85	0.58
1:F:91:ALA:HB2	1:F:310:VAL:HG11	1.84	0.58
1:C:154:VAL:O	1:C:158:VAL:HG23	2.04	0.58
1:F:217:GLY:HA2	1:F:240:THR:OG1	2.04	0.58
1:B:91:ALA:HB2	1:B:310:VAL:HG11	1.85	0.58
1:E:71:ARG:NH1	1:E:86:LYS:HE2	2.18	0.58
1:B:338:GLN:O	1:B:342:ASN:HB2	2.03	0.57
1:C:114:ASN:HD22	1:C:215:ILE:HG23	1.67	0.57
1:D:217:GLY:HA2	1:D:240:THR:OG1	2.03	0.57
1:F:403:ILE:HG13	1:F:404:ASP:N	2.18	0.57
1:A:292:PRO:HG2	1:F:365:ARG:CZ	2.34	0.57
1:D:383:THR:OG1	1:D:409:PRO:HG3	2.04	0.57
1:B:212:LEU:HD11	1:B:307:ARG:HG3	1.86	0.57
1:D:154:VAL:O	1:D:158:VAL:HG23	2.05	0.57
1:F:257:VAL:HG23	1:F:297:LYS:HD3	1.86	0.57
1:D:307:ARG:O	1:D:309:PRO:HD3	2.05	0.57
1:E:212:LEU:HD21	1:E:303:GLU:HG3	1.85	0.57
1:C:71:ARG:HH12	1:C:86:LYS:HE2	1.70	0.57
1:E:383:THR:OG1	1:E:409:PRO:HG3	2.05	0.57
1:E:117:LEU:HD23	1:E:312:ALA:HB3	1.85	0.57
1:D:212:LEU:HD11	1:D:307:ARG:HG3	1.86	0.56
1:E:154:VAL:O	1:E:158:VAL:HG23	2.05	0.56
1:B:164:LYS:HG2	1:C:209:GLN:CD	2.25	0.56
1:B:358:ILE:HD13	1:B:376:VAL:HG22	1.87	0.56
1:C:217:GLY:HA3	1:C:241:SER:OG	2.05	0.56
1:D:91:ALA:HB2	1:D:310:VAL:HG11	1.86	0.56
1:C:217:GLY:HA2	1:C:240:THR:OG1	2.05	0.56
1:E:319:GLU:HB3	1:E:363:MET:SD	2.45	0.56
1:C:338:GLN:O	1:C:342:ASN:HB2	2.04	0.56
1:F:154:VAL:O	1:F:158:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:212:LEU:HD21	1:F:303:GLU:CG	2.36	0.56
1:F:212:LEU:HD21	1:F:303:GLU:HG3	1.88	0.56
1:D:257:VAL:HG23	1:D:297:LYS:HD3	1.86	0.56
1:F:186:ILE:O	1:F:189:ILE:HG12	2.06	0.56
1:B:217:GLY:HA3	1:B:241:SER:OG	2.06	0.56
1:B:261:ARG:NH2	1:B:291:GLU:HG3	2.21	0.55
1:D:399:ASP:O	1:D:403:ILE:HG12	2.06	0.55
1:A:383:THR:OG1	1:A:409:PRO:HG3	2.06	0.55
1:C:282:SER:O	1:C:286:LEU:HD13	2.05	0.55
1:C:365:ARG:NH2	1:D:292:PRO:HG2	2.20	0.55
1:D:338:GLN:O	1:D:342:ASN:HB2	2.05	0.55
1:C:208:GLN:O	1:C:212:LEU:HB2	2.06	0.55
1:B:391:GLU:O	1:B:391:GLU:HG2	2.06	0.55
1:F:117:LEU:HD23	1:F:312:ALA:HB3	1.88	0.55
1:F:123:SER:HA	1:F:317:LEU:HA	1.89	0.55
1:D:391:GLU:O	1:D:391:GLU:HG2	2.06	0.55
1:E:217:GLY:HA2	1:E:240:THR:OG1	2.07	0.55
1:E:257:VAL:HG23	1:E:297:LYS:HD3	1.89	0.55
1:A:114:ASN:HD22	1:A:215:ILE:HG23	1.70	0.54
1:A:257:VAL:HG23	1:A:297:LYS:HD3	1.88	0.54
1:C:150:GLU:CA	1:C:203:SER:HB2	2.29	0.54
1:F:151:ALA:O	1:F:154:VAL:HG12	2.07	0.54
1:B:403:ILE:HG13	1:B:404:ASP:N	2.22	0.54
1:C:317:LEU:HD12	1:C:325:ILE:HD11	1.89	0.54
1:E:261:ARG:NH2	1:E:291:GLU:HG3	2.21	0.54
1:A:403:ILE:HG13	1:A:404:ASP:N	2.23	0.54
1:C:257:VAL:HG23	1:C:297:LYS:HD3	1.88	0.54
1:E:217:GLY:HA3	1:E:241:SER:OG	2.07	0.54
1:B:217:GLY:HA2	1:B:240:THR:OG1	2.07	0.54
1:E:79:ILE:HD12	1:E:325:ILE:HG12	1.89	0.54
1:A:154:VAL:O	1:A:158:VAL:HG23	2.08	0.54
1:A:391:GLU:O	1:A:391:GLU:HG2	2.06	0.54
1:E:91:ALA:HB2	1:E:310:VAL:HG11	1.90	0.54
1:E:361:LYS:HD3	1:E:403:ILE:HG22	1.90	0.54
1:E:212:LEU:HD21	1:E:303:GLU:CG	2.38	0.54
1:E:174:GLN:O	1:E:178:ARG:HG3	2.08	0.54
1:C:399:ASP:O	1:C:403:ILE:HG12	2.08	0.54
1:D:354:ALA:O	1:D:358:ILE:HG13	2.07	0.54
1:A:327:LYS:HD2	1:A:355:LEU:HD13	1.90	0.53
1:C:383:THR:OG1	1:C:409:PRO:HG3	2.08	0.53
1:F:383:THR:OG1	1:F:409:PRO:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:VAL:HG23	1:B:297:LYS:HD3	1.90	0.53
1:C:403:ILE:HG13	1:C:404:ASP:N	2.21	0.53
1:B:307:ARG:O	1:B:309:PRO:HD3	2.08	0.53
1:D:403:ILE:HG13	1:D:404:ASP:N	2.23	0.53
1:F:217:GLY:HA3	1:F:241:SER:OG	2.09	0.53
1:F:354:ALA:O	1:F:358:ILE:HG13	2.08	0.53
1:F:212:LEU:CD1	1:F:307:ARG:HG3	2.39	0.53
1:C:212:LEU:HD11	1:C:307:ARG:HG3	1.91	0.53
1:F:321:ALA:O	1:F:325:ILE:HG13	2.09	0.53
1:A:212:LEU:CD1	1:A:307:ARG:HG3	2.38	0.53
1:B:322:LEU:HD23	1:B:325:ILE:HD12	1.91	0.53
1:E:391:GLU:HG2	1:E:391:GLU:O	2.08	0.52
1:F:136:LEU:O	1:F:138:VAL:HG23	2.08	0.52
1:D:261:ARG:NH2	1:D:291:GLU:HG3	2.25	0.52
1:F:190:SER:HB2	1:F:299:GLY:HA3	1.92	0.52
1:E:321:ALA:O	1:E:325:ILE:HG13	2.10	0.52
1:E:123:SER:HA	1:E:317:LEU:HD23	1.90	0.52
1:E:190:SER:HB2	1:E:299:GLY:HA3	1.91	0.52
1:F:391:GLU:O	1:F:391:GLU:HG2	2.10	0.52
1:A:321:ALA:O	1:A:325:ILE:HG13	2.10	0.52
1:C:251:PHE:HB3	1:C:254:LEU:HB2	1.92	0.52
1:D:217:GLY:HA3	1:D:241:SER:OG	2.10	0.52
1:C:91:ALA:HB2	1:C:310:VAL:HG11	1.91	0.51
1:D:76:ASP:CB	1:D:330:LYS:HE3	2.37	0.51
1:C:148:LEU:O	1:C:154:VAL:HG11	2.10	0.51
1:A:373:ARG:CZ	1:B:111:GLY:HA2	2.41	0.51
1:E:344:GLU:OE2	1:F:93:TYR:HE1	1.94	0.51
1:F:261:ARG:NH2	1:F:291:GLU:HG3	2.26	0.51
1:C:149:THR:HA	1:C:207:VAL:HG21	1.92	0.51
1:B:396:VAL:HB	1:B:410:LEU:HB3	1.91	0.51
1:D:114:ASN:HD22	1:D:215:ILE:HG23	1.75	0.51
1:F:71:ARG:HA	1:F:74:LEU:HD12	1.93	0.51
1:A:91:ALA:HB2	1:A:310:VAL:HG11	1.91	0.50
1:C:212:LEU:HD21	1:C:303:GLU:HG3	1.93	0.50
1:B:251:PHE:HB3	1:B:254:LEU:HB2	1.93	0.50
1:B:385:TYR:OH	1:C:71:ARG:HD3	2.11	0.50
1:B:410:LEU:HD12	1:B:411:LEU:N	2.27	0.50
1:D:186:ILE:O	1:D:189:ILE:HG12	2.10	0.50
1:C:212:LEU:HD21	1:C:303:GLU:CG	2.41	0.50
1:A:117:LEU:HD23	1:A:312:ALA:HB3	1.93	0.50
1:B:186:ILE:O	1:B:189:ILE:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:LEU:O	1:D:154:VAL:HG11	2.11	0.50
1:D:212:LEU:HD21	1:D:303:GLU:CG	2.42	0.50
1:D:307:ARG:C	1:D:309:PRO:HD3	2.32	0.50
1:F:346:VAL:HG13	1:F:394:GLU:HA	1.94	0.50
1:B:138:VAL:HG13	1:B:179:GLY:HA2	1.94	0.50
1:E:149:THR:HA	1:E:207:VAL:HG21	1.94	0.50
1:E:236:LEU:O	1:E:237:GLN:HG2	2.12	0.50
1:A:212:LEU:HD21	1:A:303:GLU:CG	2.42	0.50
1:A:217:GLY:HA3	1:A:241:SER:OG	2.09	0.50
1:B:86:LYS:O	1:B:90:VAL:HG23	2.12	0.50
1:D:251:PHE:HB3	1:D:254:LEU:HB2	1.93	0.50
1:F:327:LYS:HD2	1:F:355:LEU:HD13	1.93	0.50
1:A:251:PHE:HB3	1:A:254:LEU:HB2	1.93	0.49
1:A:186:ILE:O	1:A:189:ILE:HG12	2.12	0.49
1:B:386:ASP:HB3	1:C:68:HIS:NE2	2.27	0.49
1:F:307:ARG:C	1:F:309:PRO:HD3	2.32	0.49
1:C:117:LEU:HD23	1:C:312:ALA:HB3	1.93	0.49
1:D:365:ARG:NH1	1:D:375:ILE:HG12	2.27	0.49
1:B:76:ASP:CB	1:B:330:LYS:HE3	2.37	0.49
1:B:307:ARG:C	1:B:309:PRO:HD3	2.32	0.49
1:E:251:PHE:HB3	1:E:254:LEU:HB2	1.93	0.49
1:B:200:ARG:HD2	1:B:200:ARG:N	2.27	0.49
1:C:261:ARG:NH2	1:C:291:GLU:HG3	2.27	0.49
1:F:251:PHE:HB3	1:F:254:LEU:HB2	1.94	0.49
1:C:186:ILE:O	1:C:189:ILE:HG12	2.13	0.49
1:D:146:THR:O	1:D:149:THR:HG22	2.13	0.49
1:D:406:GLN:HG3	1:D:407:SER:N	2.28	0.49
1:A:365:ARG:NH1	1:A:375:ILE:HG12	2.27	0.49
1:B:212:LEU:CD1	1:B:307:ARG:HG3	2.42	0.49
1:C:71:ARG:NH1	1:C:86:LYS:HE2	2.28	0.49
1:E:212:LEU:CD1	1:E:307:ARG:HG3	2.43	0.49
1:E:381:LEU:HD11	1:F:86:LYS:CD	2.42	0.49
1:E:200:ARG:N	1:E:200:ARG:HD2	2.28	0.48
1:A:236:LEU:O	1:A:237:GLN:HG2	2.12	0.48
1:D:212:LEU:CD1	1:D:307:ARG:HG3	2.43	0.48
1:F:307:ARG:O	1:F:309:PRO:HD3	2.13	0.48
1:B:209:GLN:O	1:B:212:LEU:HB3	2.13	0.48
1:C:160:ASN:O	1:C:163:GLN:HG2	2.13	0.48
1:D:138:VAL:HG13	1:D:179:GLY:HA2	1.93	0.48
1:E:186:ILE:O	1:E:189:ILE:HG12	2.14	0.48
1:F:282:SER:O	1:F:286:LEU:HD13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:LEU:CD1	1:C:86:LYS:HD2	2.42	0.48
1:D:190:SER:HB2	1:D:299:GLY:HA3	1.96	0.48
1:E:108:VAL:HG12	1:E:109:GLU:N	2.28	0.48
1:E:327:LYS:HD2	1:E:355:LEU:HD13	1.96	0.48
1:C:212:LEU:CD1	1:C:307:ARG:HG3	2.44	0.48
1:E:251:PHE:HB3	1:E:254:LEU:CB	2.43	0.48
1:D:212:LEU:HD21	1:D:303:GLU:HG3	1.96	0.48
1:A:160:ASN:O	1:A:163:GLN:HG2	2.14	0.48
1:C:307:ARG:C	1:C:309:PRO:HD3	2.35	0.48
1:E:307:ARG:C	1:E:309:PRO:HD3	2.34	0.48
1:B:408:GLU:HB3	1:B:409:PRO:HD2	1.95	0.48
1:D:236:LEU:O	1:D:237:GLN:HB2	2.14	0.48
1:E:319:GLU:O	1:E:323:ILE:HG13	2.13	0.48
1:F:104:THR:CB	1:F:108:VAL:HB	2.43	0.48
1:A:261:ARG:NH2	1:A:291:GLU:HG3	2.28	0.47
1:D:98:ARG:HD2	1:D:110:LEU:CB	2.44	0.47
1:A:212:LEU:HD21	1:A:303:GLU:HG3	1.96	0.47
1:A:282:SER:O	1:A:286:LEU:HD13	2.15	0.47
1:F:317:LEU:CD1	1:F:368:GLY:HA2	2.44	0.47
1:B:371:GLY:O	1:B:375:ILE:HG13	2.15	0.47
1:C:120:PRO:HG2	1:C:316:GLU:HG2	1.96	0.47
1:D:347:ASP:O	1:D:394:GLU:HB2	2.14	0.47
1:E:114:ASN:HD22	1:E:215:ILE:HG23	1.78	0.47
1:C:365:ARG:HH21	1:D:292:PRO:HG2	1.79	0.47
1:E:148:LEU:O	1:E:154:VAL:HG11	2.14	0.47
1:F:387:LEU:HD13	1:F:395:LYS:HE3	1.97	0.47
1:E:282:SER:O	1:E:286:LEU:HD13	2.15	0.47
1:A:138:VAL:HG13	1:A:179:GLY:HA2	1.97	0.47
1:C:236:LEU:O	1:C:237:GLN:HB3	2.15	0.47
1:E:136:LEU:O	1:E:138:VAL:HG23	2.15	0.47
1:E:150:GLU:HA	1:E:203:SER:CB	2.34	0.46
1:E:160:ASN:O	1:E:163:GLN:HG2	2.15	0.46
1:B:160:ASN:O	1:B:163:GLN:HG2	2.15	0.46
1:D:138:VAL:CG1	1:D:179:GLY:HA2	2.45	0.46
1:D:88:LEU:HD23	1:D:115:ILE:HD13	1.97	0.46
1:A:251:PHE:HB3	1:A:254:LEU:CB	2.45	0.46
1:B:150:GLU:HA	1:B:203:SER:CB	2.39	0.46
1:C:328:GLU:HB2	1:C:329:PRO:HD3	1.96	0.46
1:B:212:LEU:HD21	1:B:303:GLU:CG	2.46	0.46
1:C:104:THR:CB	1:C:108:VAL:HB	2.46	0.46
1:F:365:ARG:NH1	1:F:375:ILE:HG12	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ARG:HG2	1:B:309:PRO:HB3	1.97	0.46
1:B:146:THR:O	1:B:149:THR:HG22	2.16	0.46
1:C:150:GLU:HA	1:C:203:SER:CB	2.30	0.46
1:D:251:PHE:HB3	1:D:254:LEU:CB	2.45	0.46
1:A:354:ALA:O	1:A:358:ILE:HG13	2.16	0.46
1:B:148:LEU:O	1:B:154:VAL:HG11	2.16	0.46
1:B:282:SER:O	1:B:286:LEU:HD13	2.16	0.46
1:C:373:ARG:HG2	1:D:309:PRO:HB3	1.97	0.46
1:A:138:VAL:CG1	1:A:179:GLY:HA2	2.46	0.46
1:B:138:VAL:CG1	1:B:179:GLY:HA2	2.46	0.46
1:E:182:TYR:HA	1:E:246:ILE:O	2.16	0.46
1:F:395:LYS:NZ	1:F:411:LEU:HD22	2.31	0.46
1:C:125:LYS:HB2	2:C:501:SO4:O2	2.15	0.46
1:F:361:LYS:HB2	1:F:375:ILE:HD13	1.98	0.46
1:C:343:LEU:HD13	1:D:97:LYS:HE3	1.98	0.45
1:D:190:SER:HA	1:D:208:GLN:NE2	2.31	0.45
1:F:353:GLU:CD	1:F:353:GLU:H	2.19	0.45
1:A:110:LEU:HA	1:F:336:GLN:CD	2.37	0.45
1:B:98:ARG:HD2	1:B:110:LEU:CB	2.46	0.45
1:B:141:THR:HG22	1:B:165:LEU:HD13	1.98	0.45
1:A:144:ASP:OD2	1:A:146:THR:HB	2.15	0.45
1:C:73:HIS:HB2	1:C:135:LEU:HD13	1.99	0.45
1:E:381:LEU:HD11	1:F:86:LYS:HD2	1.98	0.45
1:B:236:LEU:O	1:B:237:GLN:HB3	2.16	0.45
1:A:200:ARG:HD2	1:A:200:ARG:N	2.31	0.45
1:B:212:LEU:HD21	1:B:303:GLU:HG3	1.99	0.45
1:A:358:ILE:HD13	1:A:376:VAL:HG22	1.98	0.45
1:F:112:LYS:CE	1:F:307:ARG:HE	2.23	0.45
1:E:357:ALA:O	1:E:361:LYS:HG2	2.17	0.45
1:F:138:VAL:HG13	1:F:179:GLY:HA2	1.99	0.45
1:B:172:ASP:OD1	1:B:174:GLN:HG2	2.17	0.45
1:E:358:ILE:HD13	1:E:376:VAL:HG22	1.99	0.45
1:C:81:GLN:NE2	1:C:314:LEU:HB3	2.31	0.44
1:D:282:SER:O	1:D:286:LEU:HD13	2.17	0.44
1:B:365:ARG:NH1	1:B:375:ILE:HG12	2.32	0.44
1:A:309:PRO:HA	1:F:374:SER:HB3	1.99	0.44
1:B:149:THR:HA	1:B:207:VAL:HG21	1.99	0.44
1:C:146:THR:HG23	1:D:218:THR:HG22	1.99	0.44
1:C:358:ILE:HD13	1:C:376:VAL:HG22	1.98	0.44
1:A:77:TYR:CE2	1:A:330:LYS:HD2	2.52	0.44
1:E:295:LEU:HB2	1:E:305:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:ALA:CB	1:C:140:PHE:HB2	2.46	0.44
1:C:347:ASP:O	1:C:394:GLU:HB2	2.18	0.44
1:E:83:GLN:O	1:E:87:VAL:HG23	2.18	0.44
1:E:173:VAL:HG13	1:E:238:VAL:HG22	1.99	0.44
1:F:251:PHE:HB3	1:F:254:LEU:CB	2.47	0.44
1:B:73:HIS:HB2	1:B:135:LEU:HD13	1.99	0.44
1:E:354:ALA:O	1:E:358:ILE:HG13	2.18	0.44
1:A:377:GLU:OE1	1:B:309:PRO:HB2	2.17	0.44
1:E:151:ALA:O	1:E:154:VAL:HG12	2.18	0.44
1:E:157:ASP:O	1:E:160:ASN:HB3	2.17	0.44
1:F:169:CYS:SG	1:F:175:LYS:HB2	2.58	0.44
1:C:251:PHE:HB3	1:C:254:LEU:CB	2.47	0.44
1:F:160:ASN:O	1:F:163:GLN:HG2	2.17	0.44
1:A:217:GLY:HA3	1:A:241:SER:HG	1.82	0.44
1:C:346:VAL:HG13	1:C:394:GLU:HA	1.99	0.44
1:C:387:LEU:C	1:C:389:SER:H	2.21	0.44
1:D:150:GLU:HA	1:D:203:SER:CB	2.37	0.44
1:D:381:LEU:CD1	1:E:86:LYS:HD2	2.39	0.44
1:B:251:PHE:HB3	1:B:254:LEU:CB	2.48	0.43
1:D:151:ALA:O	1:D:154:VAL:HG12	2.17	0.43
1:E:209:GLN:O	1:E:212:LEU:HB3	2.18	0.43
1:A:171:TYR:HH	1:B:235:PHE:HD1	1.65	0.43
1:A:346:VAL:HG13	1:A:394:GLU:HA	2.01	0.43
1:B:136:LEU:O	1:B:138:VAL:HG23	2.18	0.43
1:C:190:SER:HB2	1:C:299:GLY:HA3	1.99	0.43
1:F:320:GLU:HG3	1:F:324:GLN:HE21	1.83	0.43
1:A:77:TYR:CZ	1:A:330:LYS:HD2	2.53	0.43
1:C:157:ASP:O	1:C:160:ASN:HB3	2.18	0.43
1:C:295:LEU:HB2	1:C:305:ILE:HD13	2.01	0.43
1:D:388:PRO:HB2	1:E:66:THR:HG22	1.99	0.43
1:B:190:SER:HB2	1:B:299:GLY:HA3	2.00	0.43
1:C:307:ARG:O	1:C:309:PRO:HD3	2.18	0.43
1:F:141:THR:HG22	1:F:165:LEU:HD13	2.00	0.43
1:F:327:LYS:O	1:F:335:LYS:HE3	2.18	0.43
1:B:237:GLN:O	1:B:237:GLN:HG2	2.18	0.43
1:A:307:ARG:C	1:A:309:PRO:HD3	2.38	0.43
1:F:88:LEU:CD2	1:F:115:ILE:HG21	2.49	0.43
1:D:149:THR:HA	1:D:207:VAL:HG21	2.00	0.43
1:E:88:LEU:HD23	1:E:115:ILE:HD13	2.00	0.43
1:F:358:ILE:HD13	1:F:376:VAL:HG22	2.01	0.43
1:A:309:PRO:HB2	1:F:377:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237:GLN:O	1:F:237:GLN:HG2	2.19	0.43
1:D:128:LEU:O	1:D:132:LEU:HG	2.19	0.42
1:E:163:GLN:HE22	1:F:202:VAL:HG13	1.84	0.42
1:E:358:ILE:HG12	1:E:402:VAL:HG11	2.01	0.42
1:B:112:LYS:CE	1:B:307:ARG:HE	2.25	0.42
1:B:169:CYS:SG	1:B:175:LYS:HB2	2.59	0.42
1:C:151:ALA:O	1:C:154:VAL:HG12	2.19	0.42
1:C:172:ASP:OD1	1:C:174:GLN:HG2	2.19	0.42
1:B:83:GLN:O	1:B:87:VAL:HG23	2.19	0.42
1:B:410:LEU:HD12	1:B:411:LEU:H	1.83	0.42
1:D:371:GLY:O	1:D:375:ILE:HG13	2.18	0.42
1:F:295:LEU:HB2	1:F:305:ILE:HD13	2.01	0.42
1:A:136:LEU:O	1:A:138:VAL:HG23	2.18	0.42
1:A:157:ASP:O	1:A:160:ASN:HB3	2.20	0.42
1:A:371:GLY:O	1:A:375:ILE:HG13	2.19	0.42
1:C:136:LEU:O	1:C:138:VAL:HG23	2.18	0.42
1:F:387:LEU:HD13	1:F:395:LYS:CE	2.49	0.42
1:B:131:THR:O	1:B:135:LEU:HG	2.20	0.42
1:C:361:LYS:HB2	1:C:375:ILE:HD13	2.00	0.42
1:E:133:ALA:CB	1:E:140:PHE:HB2	2.50	0.42
1:F:114:ASN:HD22	1:F:215:ILE:HG23	1.83	0.42
1:A:73:HIS:HB2	1:A:135:LEU:HD13	2.01	0.42
1:A:190:SER:HB2	1:A:299:GLY:HA3	2.01	0.42
1:B:64:LEU:HA	1:B:65:PRO:HD3	1.80	0.42
1:B:301:ILE:HG13	1:B:304:PHE:H	1.85	0.42
1:C:174:GLN:HG3	1:C:175:LYS:N	2.34	0.42
1:E:138:VAL:CG1	1:E:179:GLY:HA2	2.50	0.42
1:F:209:GLN:O	1:F:212:LEU:HB3	2.19	0.42
1:D:79:ILE:HD13	1:D:324:GLN:HB3	2.02	0.42
1:E:190:SER:HA	1:E:208:GLN:NE2	2.35	0.42
1:F:172:ASP:OD1	1:F:174:GLN:HG2	2.20	0.42
1:C:149:THR:HA	1:C:207:VAL:CG2	2.50	0.42
1:C:357:ALA:O	1:C:361:LYS:HG2	2.20	0.42
1:C:354:ALA:O	1:C:358:ILE:HG13	2.20	0.42
1:B:317:LEU:HD13	1:B:325:ILE:HD11	2.01	0.41
1:E:167:GLN:HA	1:E:171:TYR:CE1	2.55	0.41
1:C:138:VAL:HG13	1:C:179:GLY:HA2	2.02	0.41
1:C:195:ASN:N	1:C:196:PRO:HD3	2.35	0.41
1:D:148:LEU:CA	1:D:154:VAL:HG21	2.44	0.41
1:A:92:VAL:HG11	1:A:136:LEU:HD11	2.01	0.41
1:B:119:GLY:O	1:B:250:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:VAL:HB	1:D:410:LEU:HB3	2.02	0.41
1:E:73:HIS:HB2	1:E:135:LEU:HD13	2.01	0.41
1:E:371:GLY:O	1:E:375:ILE:HG13	2.20	0.41
1:A:295:LEU:HB2	1:A:305:ILE:HD13	2.02	0.41
1:A:296:ILE:HD11	1:A:302:PRO:HA	2.02	0.41
1:A:301:ILE:HG13	1:A:304:PHE:H	1.85	0.41
1:B:331:ASN:ND2	1:C:109:GLU:HG3	2.35	0.41
1:E:214:LEU:HD23	1:E:214:LEU:HA	1.93	0.41
1:A:369:ALA:HA	1:A:372:LEU:HG	2.03	0.41
1:C:383:THR:O	1:C:387:LEU:HB2	2.19	0.41
1:D:169:CYS:SG	1:D:175:LYS:HB2	2.60	0.41
1:F:317:LEU:HD13	1:F:368:GLY:HA2	2.01	0.41
1:A:148:LEU:CA	1:A:154:VAL:HG21	2.46	0.41
1:B:157:ASP:O	1:B:160:ASN:HB3	2.20	0.41
1:E:169:CYS:SG	1:E:172:ASP:HB3	2.60	0.41
1:C:327:LYS:O	1:C:335:LYS:HE3	2.21	0.41
1:D:328:GLU:HB2	1:D:329:PRO:HD3	2.03	0.41
1:E:331:ASN:ND2	1:F:109:GLU:HG3	2.36	0.41
1:F:66:THR:OG1	1:F:69:GLU:HG3	2.20	0.41
1:F:292:PRO:O	1:F:296:ILE:HG12	2.20	0.41
1:F:371:GLY:O	1:F:375:ILE:HG13	2.20	0.41
1:C:174:GLN:O	1:C:178:ARG:HG3	2.21	0.41
1:D:346:VAL:HG13	1:D:394:GLU:HA	2.03	0.41
1:F:387:LEU:CB	1:F:388:PRO:HD3	2.51	0.41
1:E:303:GLU:HA	1:E:303:GLU:OE1	2.20	0.41
1:A:133:ALA:CB	1:A:140:PHE:HB2	2.51	0.40
1:B:346:VAL:HG21	1:B:387:LEU:HD11	2.03	0.40
1:C:254:LEU:O	1:C:258:ILE:HG13	2.21	0.40
1:C:138:VAL:CG1	1:C:179:GLY:HA2	2.50	0.40
1:E:307:ARG:O	1:E:309:PRO:HD3	2.21	0.40
1:A:98:ARG:HD2	1:A:110:LEU:CB	2.51	0.40
1:B:116:LEU:HD12	1:B:247:CYS:O	2.22	0.40
1:F:128:LEU:O	1:F:132:LEU:HG	2.21	0.40
1:F:408:GLU:HB3	1:F:409:PRO:HD2	2.03	0.40
1:A:361:LYS:HB2	1:A:375:ILE:HD13	2.04	0.40
1:C:190:SER:HA	1:C:208:GLN:NE2	2.37	0.40
1:D:64:LEU:HA	1:D:65:PRO:HD3	1.80	0.40
1:D:295:LEU:HB2	1:D:305:ILE:HD13	2.01	0.40
1:E:138:VAL:HG13	1:E:179:GLY:HA2	2.03	0.40
1:F:138:VAL:CG1	1:F:179:GLY:HA2	2.52	0.40
1:A:357:ALA:O	1:A:361:LYS:HG2	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	297/363 (82%)	284 (96%)	13 (4%)	0	100	100
1	B	298/363 (82%)	283 (95%)	15 (5%)	0	100	100
1	C	309/363 (85%)	289 (94%)	20 (6%)	0	100	100
1	D	294/363 (81%)	279 (95%)	15 (5%)	0	100	100
1	E	310/363 (85%)	293 (94%)	17 (6%)	0	100	100
1	F	300/363 (83%)	283 (94%)	17 (6%)	0	100	100
All	All	1808/2178 (83%)	1711 (95%)	97 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	240/299 (80%)	240 (100%)	0	100	100
1	B	240/299 (80%)	240 (100%)	0	100	100
1	C	239/299 (80%)	239 (100%)	0	100	100
1	D	240/299 (80%)	240 (100%)	0	100	100
1	E	242/299 (81%)	242 (100%)	0	100	100
1	F	240/299 (80%)	240 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1441/1794 (80%)	1441 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	B	68	HIS
1	B	114	ASN
1	C	73	HIS
1	D	114	ASN
1	E	73	HIS
1	E	114	ASN
1	E	209	GLN
1	F	114	ASN
1	F	324	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	501	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	E	501	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	F	501	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	501	-	4,4,4	0.14	0	6,6,6	0.04	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.

1 monomer is involved in 1 short contact:

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	309/363 (85%)	0.40	17 (5%)	25	22	176, 221, 267, 325	0
1	B	308/363 (84%)	0.13	10 (3%)	47	37	175, 216, 300, 377	0
1	C	317/363 (87%)	0.38	25 (7%)	12	11	144, 208, 331, 421	0
1	D	304/363 (83%)	0.18	13 (4%)	35	29	151, 195, 302, 370	0
1	E	318/363 (87%)	0.17	13 (4%)	37	30	177, 231, 301, 357	0
1	F	310/363 (85%)	0.19	16 (5%)	27	24	168, 214, 290, 348	0
All	All	1866/2178 (85%)	0.24	94 (5%)	28	25	144, 218, 301, 421	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	105	SER	8.8
1	A	265	GLY	8.7
1	A	266	SER	7.3
1	B	200	ARG	7.0
1	A	264	THR	6.7
1	F	106	ASN	6.4
1	C	195	ASN	5.3
1	C	105	SER	4.9
1	B	203	SER	4.8
1	D	281	ALA	4.8
1	C	265	GLY	4.7
1	F	107	GLY	4.6
1	C	104	THR	4.6
1	C	101	ASN	4.6
1	B	266	SER	4.4
1	F	264	THR	4.4
1	E	196	PRO	4.4
1	C	266	SER	4.3
1	F	104	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	103	ASP	4.2
1	D	394	GLU	4.1
1	C	237	GLN	4.0
1	C	238	VAL	3.9
1	E	266	SER	3.8
1	F	265	GLY	3.7
1	C	103	ASP	3.6
1	E	150	GLU	3.6
1	C	106	ASN	3.5
1	A	103	ASP	3.5
1	D	152	GLY	3.5
1	E	149	THR	3.4
1	C	102	GLY	3.4
1	F	171	TYR	3.4
1	A	106	ASN	3.3
1	A	200	ARG	3.3
1	B	289	GLN	3.3
1	C	149	THR	3.3
1	C	196	PRO	3.3
1	D	150	GLU	3.2
1	B	204	GLY	3.2
1	A	411	LEU	3.2
1	B	201	ASP	3.1
1	B	218	THR	3.1
1	F	73	HIS	3.0
1	D	151	ALA	3.0
1	D	235	PHE	3.0
1	C	150	GLU	3.0
1	D	392	ASP	2.9
1	E	265	GLY	2.9
1	E	200	ARG	2.9
1	A	392	ASP	2.9
1	D	203	SER	2.9
1	C	109	GLU	2.8
1	C	100	ARG	2.8
1	A	237	GLN	2.8
1	F	202	VAL	2.7
1	F	263	GLU	2.7
1	E	173	VAL	2.7
1	D	264	THR	2.7
1	F	103	ASP	2.7
1	F	201	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	238	VAL	2.6
1	D	390	MET	2.6
1	B	150	GLU	2.6
1	C	137	ASP	2.6
1	C	156	GLU	2.5
1	B	392	ASP	2.5
1	C	392	ASP	2.4
1	E	79	ILE	2.4
1	D	201	ASP	2.4
1	E	174	GLN	2.4
1	A	351	ARG	2.4
1	C	142	MET	2.4
1	A	350	PHE	2.3
1	F	76	ASP	2.3
1	C	236	LEU	2.3
1	E	106	ASN	2.3
1	C	170	ASP	2.3
1	A	281	ALA	2.3
1	E	100	ARG	2.3
1	F	172	ASP	2.3
1	E	201	ASP	2.2
1	A	409	PRO	2.2
1	A	344	GLU	2.1
1	F	259	SER	2.1
1	C	158	VAL	2.1
1	C	171	TYR	2.1
1	A	156	GLU	2.1
1	A	319	GLU	2.1
1	C	159	GLU	2.1
1	E	78	VAL	2.1
1	D	156	GLU	2.1
1	F	162	ILE	2.0
1	B	258	ILE	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 monosaccharides 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(Å^2)	Q<0.9
2	SO4	B	501	5/5	0.71	0.43	201,205,209,212	0
2	SO4	D	501	5/5	0.81	0.39	194,195,199,206	0
2	SO4	F	501	5/5	0.90	0.17	174,177,179,180	0
2	SO4	E	501	5/5	0.92	0.39	204,204,209,215	0
2	SO4	A	501	5/5	0.95	0.23	203,210,212,216	0
2	SO4	C	501	5/5	0.96	0.12	161,161,162,168	0

6.5 Other polymers (i)

There are no such residues in this entry.