Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 06:37 AM EDT

PDB ID	:	4I63
Title	:	Crystal Structure of E-R ClpX Hexamer
Authors	:	Glynn, S.E.; Nager, A.R.; Stinson, B.S.; Schmitz, K.R.; Baker, T.A.; Sauer, R.T.
Deposited on	:	2012-11-29
Resolution	:	5.71 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:

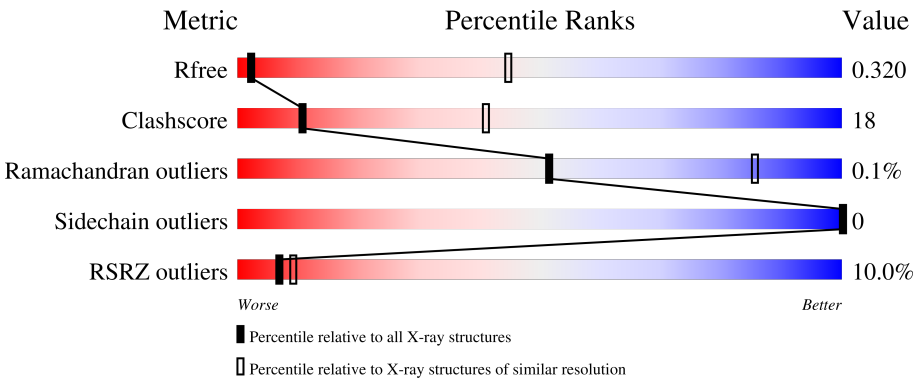
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 5.71 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	1003 (7.54-3.86)
Clashscore	141614	1028 (7.50-3.90)
Ramachandran outliers	138981	1011 (7.54-3.84)
Sidechain outliers	138945	1002 (7.58-3.82)
RSRZ outliers	127900	1002 (7.60-3.78)

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	11% 53% 33% 14%
1	B	363	9% 52% 32% 15%
1	C	363	9% 53% 29% 18%
1	D	363	8% 56% 29% 15%
1	E	363	8% 54% 33% 13%

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Mol	Chain	Length	Quality of chain
1	F	363	6% 55% 29% 16%

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	500	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13933 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.

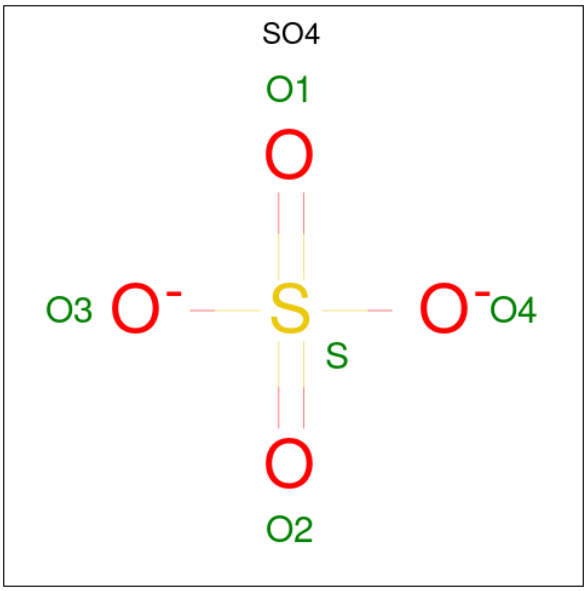
- Molecule 1 is a protein called ATP-dependent Clp protease ATP-binding subunit ClpX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	311	2332	1484	386	456	6	0	0	0
1	B	307	2304	1467	379	452	6	0	0	0
1	C	298	2273	1448	378	441	6	0	0	0
1	D	310	2317	1472	385	454	6	0	0	0
1	E	315	2356	1498	390	462	6	0	0	0
1	F	305	2321	1477	389	449	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).



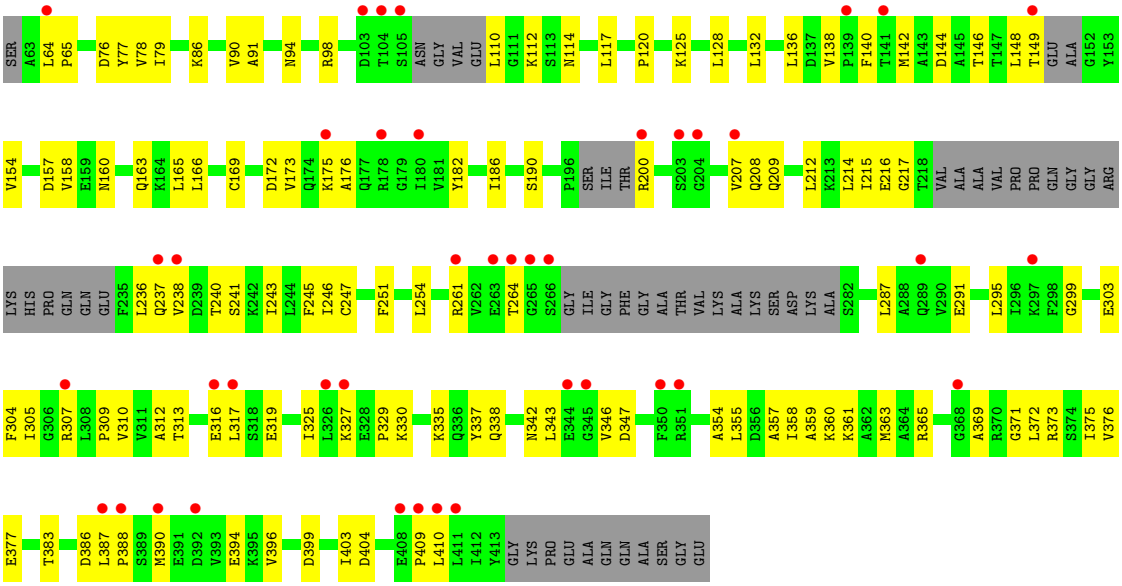
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	F	1	5	4	1	0	0

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.

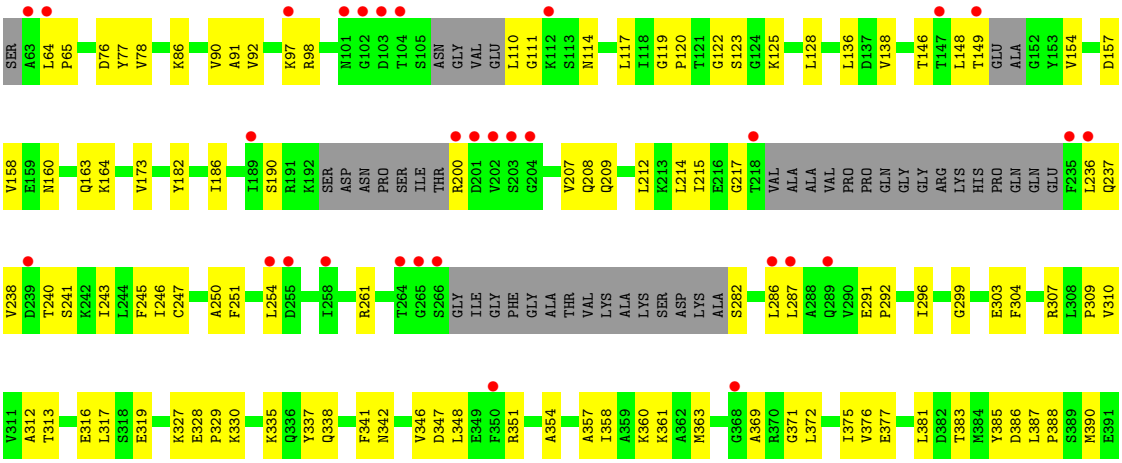
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

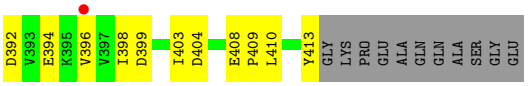
Chain A:



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

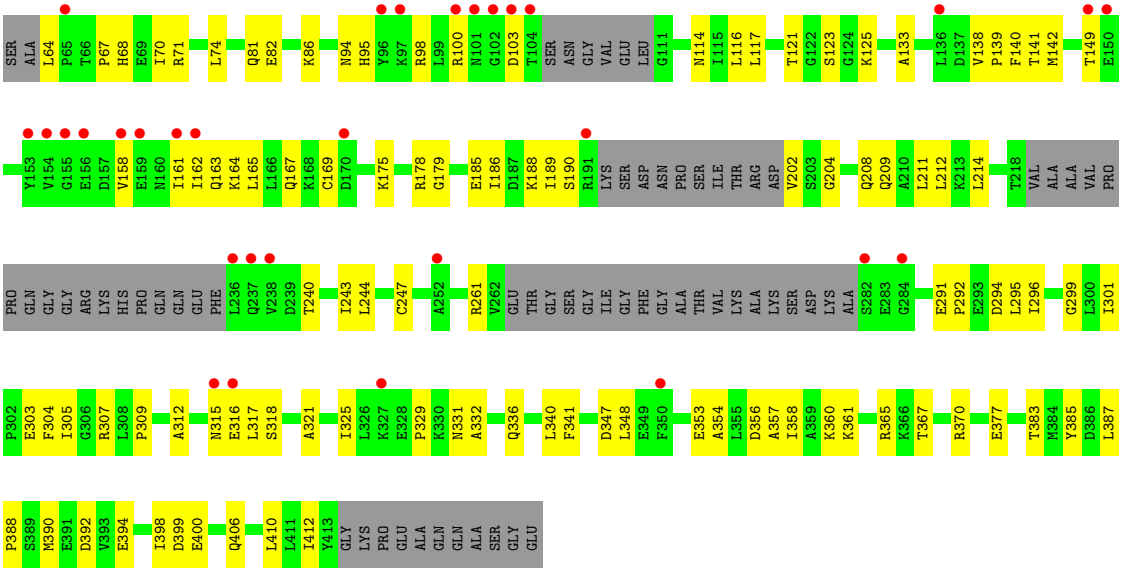
Chain B:





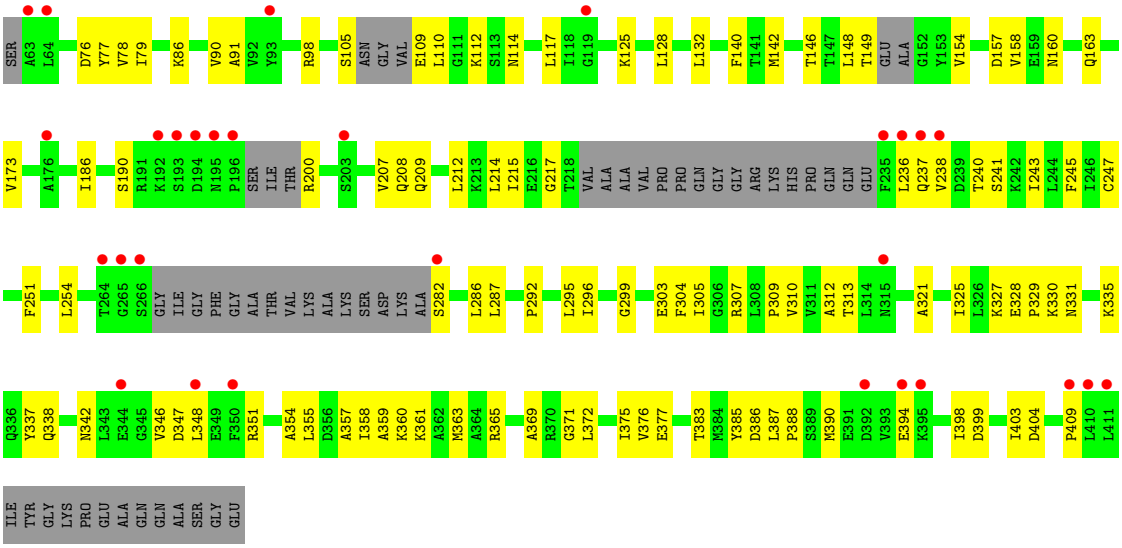
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain C:



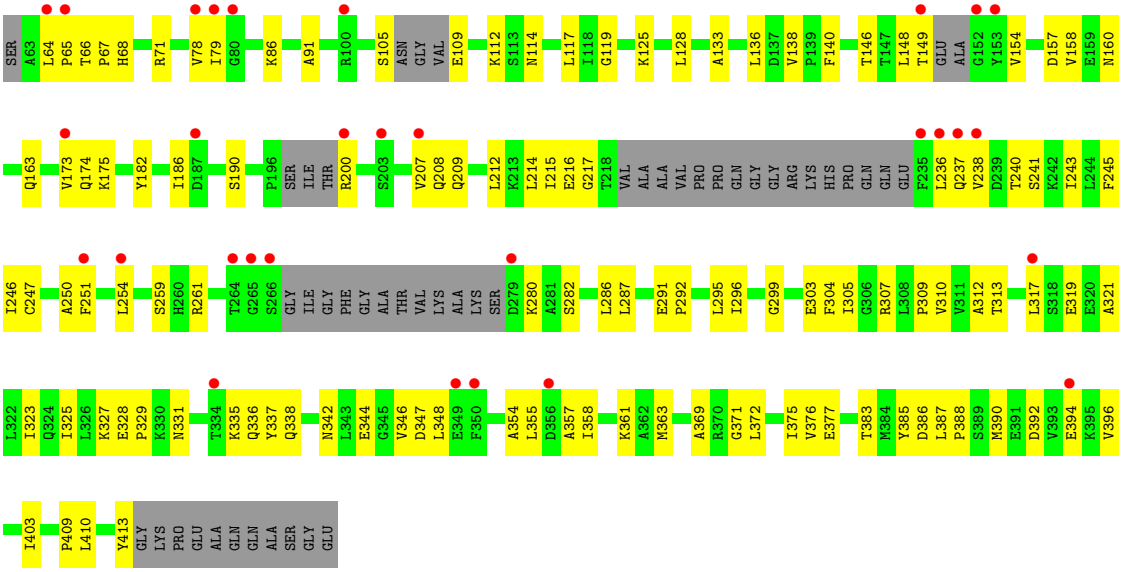
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain D:



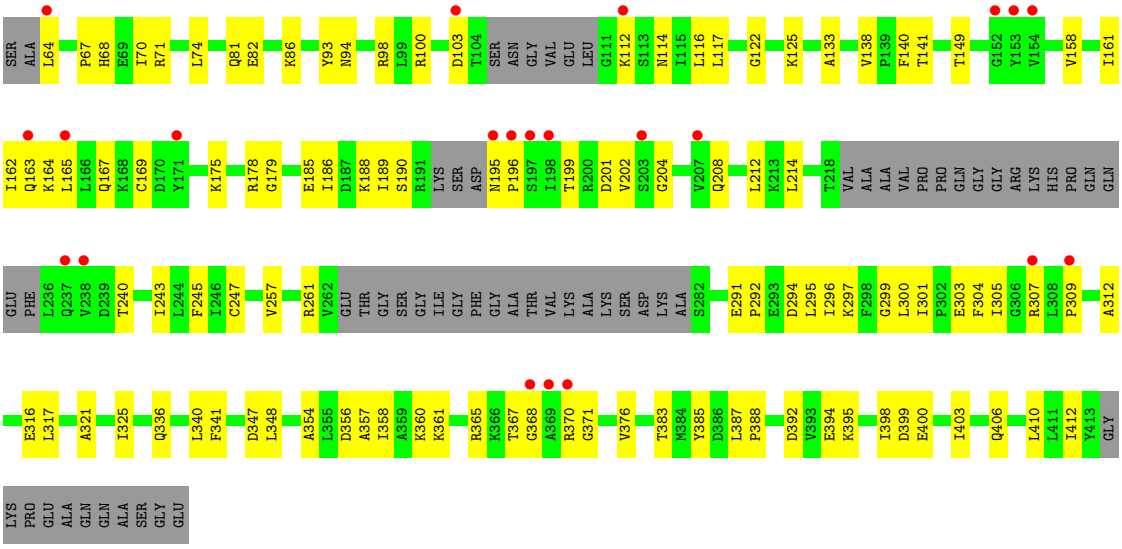
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

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	55.22Å 201.17Å 222.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.06 – 5.71 49.06 – 5.71	Depositor EDS
% Data completeness (in resolution range)	95.0 (49.06-5.71) 98.1 (49.06-5.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.28 (at 5.73Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.307 , 0.315 0.291 , 0.320	Depositor DCC
R_{free} test set	349 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å^2)	324.0	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 305.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	13933	wwPDB-VP
Average B, all atoms (Å^2)	322.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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	0/2357	0.37	0/3191
1	B	0.21	0/2328	0.38	0/3151
1	C	0.20	0/2298	0.37	0/3108
1	D	0.21	0/2341	0.37	0/3169
1	E	0.21	0/2381	0.37	0/3224
1	F	0.21	0/2347	0.37	0/3176
All	All	0.21	0/14052	0.37	0/19019

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	2332	0	2326	104	0
1	B	2304	0	2302	92	0
1	C	2273	0	2307	77	0
1	D	2317	0	2308	88	0
1	E	2356	0	2341	102	0
1	F	2321	0	2354	82	0
2	A	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	2	0
2	C	5	0	0	1	0
2	D	5	0	0	1	0
2	E	5	0	0	1	0
2	F	5	0	0	1	0
All	All	13933	0	13938	510	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 (510) 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:186:ILE:HG13	1:C:247:CYS:HB3	1.46	0.97
1:F:186:ILE:HG13	1:F:247:CYS:HB3	1.50	0.94
1:B:186:ILE:HG13	1:B:247:CYS:HB3	1.51	0.93
1:E:357:ALA:HB1	1:E:403:ILE:HG13	1.52	0.91
1:D:186:ILE:HG13	1:D:247:CYS:HB3	1.54	0.90
1:E:186:ILE:HG13	1:E:247:CYS:HB3	1.53	0.89
1:D:215:ILE:HG21	1:D:307:ARG:HB3	1.56	0.88
1:A:215:ILE:HG21	1:A:307:ARG:HB3	1.55	0.87
1:A:186:ILE:HG13	1:A:247:CYS:HB3	1.55	0.87
1:D:76:ASP:HB3	1:D:330:LYS:HE3	1.56	0.85
1:E:173:VAL:HG13	1:E:238:VAL:HG22	1.59	0.85
1:E:215:ILE:HG21	1:E:307:ARG:HB3	1.56	0.84
1:B:76:ASP:HB3	1:B:330:LYS:HE3	1.59	0.83
1:D:105:SER:HA	1:D:109:GLU:N	1.93	0.82
1:B:120:PRO:HG2	1:B:316:GLU:HA	1.62	0.81
1:A:307:ARG:HH22	1:F:370:ARG:HD2	1.47	0.80
1:C:161:ILE:HA	1:C:164:LYS:HE2	1.62	0.80
1:F:175:LYS:HD3	1:F:178:ARG:HH12	1.48	0.79
1:B:123:SER:HA	1:B:317:LEU:HD21	1.66	0.77
1:E:112:LYS:HE3	1:E:307:ARG:HE	1.48	0.77
1:A:173:VAL:HG13	1:A:238:VAL:HG22	1.66	0.76
1:F:161:ILE:HA	1:F:164:LYS:HE2	1.67	0.76
1:B:319:GLU:HB3	1:B:363:MET:SD	2.25	0.76
1:D:386:ASP:HB3	1:E:68:HIS:NE2	2.01	0.76
1:D:112:LYS:HE3	1:D:307:ARG:HE	1.50	0.76
1:F:169:CYS:SG	1:F:175:LYS:HB2	2.26	0.75
1:C:175:LYS:HD3	1:C:178:ARG:HH12	1.51	0.75
1:A:169:CYS:SG	1:A:175:LYS:HB2	2.25	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:VAL:HG13	1:D:238:VAL:HG22	1.68	0.74
1:D:214:LEU:HD22	1:D:240:THR:HG21	1.69	0.74
1:B:173:VAL:HG13	1:B:238:VAL:HG22	1.69	0.74
1:F:81:GLN:HE22	1:F:316:GLU:H	1.35	0.74
1:E:387:LEU:HB3	1:E:388:PRO:HD3	1.70	0.74
1:F:190:SER:HB2	1:F:299:GLY:HA3	1.71	0.73
1:B:337:TYR:OH	1:B:377:GLU:HG2	1.89	0.72
1:A:337:TYR:OH	1:A:377:GLU:HG2	1.90	0.72
1:C:169:CYS:SG	1:C:175:LYS:HB2	2.30	0.71
1:A:357:ALA:HB1	1:A:403:ILE:HG23	1.72	0.71
1:C:121:THR:HG21	1:C:370:ARG:HE	1.55	0.71
1:A:214:LEU:HD22	1:A:240:THR:HG21	1.72	0.71
1:D:337:TYR:OH	1:D:377:GLU:HG2	1.91	0.71
1:B:214:LEU:HD22	1:B:240:THR:HG21	1.73	0.70
1:B:357:ALA:HB1	1:B:403:ILE:HG23	1.71	0.70
1:A:359:ALA:O	1:A:363:MET:HG3	1.92	0.70
1:E:214:LEU:HD22	1:E:240:THR:HG21	1.73	0.70
1:B:387:LEU:HB3	1:B:388:PRO:HD3	1.74	0.69
1:E:337:TYR:OH	1:E:377:GLU:HG2	1.93	0.69
1:D:357:ALA:HB1	1:D:403:ILE:HG23	1.73	0.69
1:A:112:LYS:HE3	1:A:307:ARG:HE	1.58	0.68
1:C:190:SER:HB2	1:C:299:GLY:HA3	1.75	0.68
1:F:257:VAL:HG13	1:F:297:LYS:HD3	1.76	0.67
1:B:114:ASN:ND2	1:B:215:ILE:HG23	2.10	0.67
1:A:114:ASN:ND2	1:A:215:ILE:HG23	2.10	0.67
1:D:114:ASN:ND2	1:D:215:ILE:HG23	2.09	0.67
1:D:77:TYR:CZ	1:D:330:LYS:HD2	2.30	0.67
1:B:385:TYR:OH	1:C:71:ARG:HD3	1.95	0.66
1:A:365:ARG:NH2	1:B:292:PRO:HG2	2.10	0.66
1:B:148:LEU:HA	1:B:154:VAL:HG21	1.78	0.66
1:E:148:LEU:HA	1:E:154:VAL:HG21	1.77	0.66
1:C:398:ILE:HD11	1:C:410:LEU:HD11	1.77	0.66
1:E:71:ARG:HH12	1:E:86:LYS:HE2	1.59	0.66
1:A:78:VAL:HG21	1:A:128:LEU:HD23	1.78	0.66
1:D:387:LEU:HB3	1:D:388:PRO:HD3	1.75	0.66
1:A:317:LEU:HD13	1:A:325:ILE:HD11	1.78	0.65
1:E:386:ASP:HB3	1:F:68:HIS:NE2	2.10	0.65
1:A:387:LEU:HB3	1:A:388:PRO:HD3	1.79	0.65
1:E:114:ASN:ND2	1:E:215:ILE:HG23	2.13	0.65
1:B:360:LYS:HA	1:B:363:MET:HE2	1.79	0.64
1:C:385:TYR:HD1	1:D:90:VAL:HG22	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LEU:HD13	1:B:304:PHE:HA	1.80	0.64
1:B:399:ASP:O	1:B:403:ILE:HG12	1.98	0.64
1:D:359:ALA:O	1:D:363:MET:HG3	1.97	0.64
1:F:291:GLU:HG3	1:F:292:PRO:HD2	1.79	0.64
1:C:123:SER:HA	1:C:317:LEU:HD21	1.79	0.63
1:C:186:ILE:O	1:C:189:ILE:HG12	1.99	0.63
1:A:148:LEU:HA	1:A:154:VAL:HG21	1.80	0.63
1:D:148:LEU:HA	1:D:154:VAL:HG21	1.79	0.62
1:A:399:ASP:O	1:A:403:ILE:HG12	1.99	0.62
1:B:403:ILE:HG13	1:B:404:ASP:H	1.65	0.61
1:A:190:SER:HB2	1:A:299:GLY:HA3	1.83	0.60
1:A:120:PRO:HG2	1:A:316:GLU:HB2	1.83	0.60
1:F:175:LYS:HD3	1:F:178:ARG:NH1	2.15	0.60
1:E:78:VAL:HG21	1:E:128:LEU:HD23	1.84	0.60
1:C:175:LYS:HD3	1:C:178:ARG:NH1	2.16	0.60
1:A:307:ARG:HH22	1:F:370:ARG:CD	2.13	0.60
1:E:319:GLU:HG2	1:E:363:MET:SD	2.41	0.60
1:A:172:ASP:HB3	1:A:175:LYS:HG3	1.84	0.60
1:A:79:ILE:HD11	1:A:329:PRO:HD3	1.84	0.59
1:E:79:ILE:HD12	1:E:325:ILE:HG12	1.82	0.59
1:B:114:ASN:HD22	1:B:215:ILE:HG23	1.67	0.59
1:F:186:ILE:O	1:F:189:ILE:HG12	2.03	0.58
1:A:217:GLY:HA2	1:A:240:THR:OG1	2.03	0.58
1:D:383:THR:OG1	1:D:409:PRO:HG3	2.03	0.58
1:B:78:VAL:HG21	1:B:128:LEU:HD23	1.86	0.58
1:A:212:LEU:HD13	1:A:304:PHE:HA	1.86	0.58
1:D:190:SER:HB2	1:D:299:GLY:HA3	1.86	0.58
1:A:98:ARG:HD2	1:A:110:LEU:CB	2.34	0.58
1:D:78:VAL:HG21	1:D:128:LEU:HD23	1.86	0.58
1:B:261:ARG:NH2	1:B:291:GLU:HG3	2.19	0.58
1:A:125:LYS:HB2	2:A:500:SO4:O3	2.04	0.57
1:E:286:LEU:N	1:E:286:LEU:HD12	2.19	0.57
1:A:212:LEU:CD1	1:A:307:ARG:HG3	2.35	0.57
1:B:164:LYS:HE2	1:C:209:GLN:CB	2.33	0.57
1:E:71:ARG:NH1	1:E:86:LYS:HE2	2.19	0.57
1:A:373:ARG:CZ	1:B:111:GLY:HA2	2.33	0.57
1:A:403:ILE:HG13	1:A:404:ASP:H	1.69	0.57
1:A:360:LYS:HA	1:A:363:MET:HE2	1.86	0.57
1:D:212:LEU:HD13	1:D:304:PHE:HA	1.87	0.57
1:A:383:THR:OG1	1:A:409:PRO:HG3	2.05	0.57
1:D:114:ASN:HD22	1:D:215:ILE:HG23	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:LYS:HB2	2:E:500:SO4:O3	2.04	0.57
1:E:146:THR:HG21	1:F:297:LYS:HE2	1.85	0.57
1:D:125:LYS:HB2	2:D:500:SO4:O3	2.05	0.57
1:A:319:GLU:HB3	1:A:363:MET:SD	2.45	0.56
1:D:217:GLY:HA2	1:D:240:THR:OG1	2.05	0.56
1:F:82:GLU:OE2	1:F:86:LYS:HE3	2.06	0.56
1:B:383:THR:OG1	1:B:409:PRO:HG3	2.05	0.56
1:A:172:ASP:CG	1:A:175:LYS:HG3	2.26	0.56
1:A:117:LEU:HD23	1:A:312:ALA:HB3	1.88	0.56
1:C:162:ILE:HD11	1:C:214:LEU:HD11	1.88	0.56
1:E:338:GLN:O	1:E:342:ASN:HB2	2.06	0.56
1:A:287:LEU:O	1:A:313:THR:HG21	2.06	0.56
1:A:338:GLN:O	1:A:342:ASN:HB2	2.06	0.56
1:D:403:ILE:HG13	1:D:404:ASP:H	1.71	0.56
1:E:358:ILE:HD13	1:E:376:VAL:HG22	1.89	0.56
1:E:114:ASN:HD22	1:E:215:ILE:HG23	1.71	0.55
1:A:114:ASN:HD22	1:A:215:ILE:HG23	1.69	0.55
1:F:387:LEU:HB3	1:F:388:PRO:HD3	1.88	0.55
1:F:199:THR:HG22	1:F:201:ASP:H	1.71	0.55
1:B:117:LEU:HD23	1:B:312:ALA:HB3	1.88	0.55
1:D:287:LEU:O	1:D:313:THR:HG21	2.07	0.55
1:A:144:ASP:OD2	1:A:146:THR:HB	2.06	0.55
1:B:215:ILE:HG21	1:B:307:ARG:CB	2.37	0.55
1:B:217:GLY:HA3	1:B:241:SER:OG	2.07	0.55
1:D:117:LEU:HD23	1:D:312:ALA:HB3	1.89	0.55
1:E:287:LEU:O	1:E:313:THR:HG21	2.06	0.55
1:F:138:VAL:HG12	1:F:179:GLY:HA2	1.88	0.55
1:A:77:TYR:CE2	1:A:330:LYS:HD2	2.42	0.54
1:E:212:LEU:HD13	1:E:304:PHE:HA	1.88	0.54
1:D:217:GLY:HA3	1:D:241:SER:OG	2.07	0.54
1:E:190:SER:HB2	1:E:299:GLY:HA3	1.87	0.54
1:B:190:SER:HB2	1:B:299:GLY:HA3	1.89	0.54
1:C:365:ARG:HB2	1:C:367:THR:HG23	1.90	0.54
1:B:358:ILE:HD13	1:B:376:VAL:HG22	1.89	0.54
1:F:365:ARG:HB2	1:F:367:THR:HG23	1.90	0.54
1:C:291:GLU:HG3	1:C:292:PRO:HD2	1.89	0.54
1:D:360:LYS:HA	1:D:363:MET:HE2	1.89	0.54
1:A:261:ARG:NH2	1:A:291:GLU:HG3	2.23	0.54
1:A:236:LEU:O	1:A:237:GLN:HG2	2.08	0.54
1:C:392:ASP:HB2	1:C:412:ILE:O	2.08	0.54
1:D:208:GLN:O	1:D:212:LEU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:GLY:HA2	1:E:240:THR:OG1	2.08	0.54
1:F:162:ILE:HD11	1:F:214:LEU:HD11	1.90	0.54
1:E:236:LEU:O	1:E:237:GLN:HG2	2.08	0.54
1:F:357:ALA:O	1:F:361:LYS:HG2	2.08	0.54
1:B:217:GLY:HA2	1:B:240:THR:OG1	2.08	0.53
1:F:158:VAL:O	1:F:161:ILE:HG12	2.08	0.53
1:C:332:ALA:O	1:C:336:GLN:HG3	2.09	0.53
1:C:163:GLN:O	1:C:167:GLN:HG3	2.08	0.53
1:F:81:GLN:NE2	1:F:316:GLU:H	2.05	0.53
1:B:86:LYS:O	1:B:90:VAL:HG23	2.09	0.53
1:D:351:ARG:HD2	1:D:398:ILE:HG22	1.91	0.53
1:D:154:VAL:O	1:D:158:VAL:HG23	2.09	0.53
1:D:236:LEU:O	1:D:237:GLN:HG2	2.09	0.53
1:F:398:ILE:HG22	1:F:399:ASP:N	2.24	0.53
1:A:208:GLN:O	1:A:212:LEU:HB2	2.09	0.53
1:B:77:TYR:CZ	1:B:330:LYS:HD2	2.44	0.53
1:D:399:ASP:O	1:D:403:ILE:HG12	2.09	0.53
1:D:354:ALA:O	1:D:358:ILE:HG13	2.08	0.53
1:D:91:ALA:HB2	1:D:310:VAL:HG11	1.89	0.53
1:A:148:LEU:O	1:A:154:VAL:HG21	2.09	0.53
1:C:212:LEU:HD21	1:C:303:GLU:HG2	1.91	0.53
1:E:217:GLY:HA3	1:E:241:SER:OG	2.08	0.53
1:F:212:LEU:HD21	1:F:303:GLU:HG2	1.91	0.53
1:F:212:LEU:HD11	1:F:307:ARG:HG3	1.90	0.53
1:E:146:THR:CG2	1:F:297:LYS:HE2	2.39	0.52
1:E:383:THR:OG1	1:E:409:PRO:HG3	2.09	0.52
1:C:387:LEU:HB3	1:C:388:PRO:HD3	1.91	0.52
1:E:208:GLN:O	1:E:212:LEU:HB2	2.09	0.52
1:A:217:GLY:HA3	1:A:241:SER:HG	1.74	0.52
1:A:307:ARG:NH2	1:F:370:ARG:HD2	2.20	0.52
1:E:361:LYS:HB2	1:E:375:ILE:HD13	1.91	0.52
1:A:172:ASP:CB	1:A:175:LYS:HG3	2.40	0.52
1:F:392:ASP:HB2	1:F:412:ILE:O	2.10	0.52
1:C:158:VAL:O	1:C:161:ILE:HG12	2.09	0.52
1:C:212:LEU:HD11	1:C:307:ARG:HG3	1.92	0.52
1:E:388:PRO:HG2	1:F:67:PRO:CD	2.40	0.52
1:E:261:ARG:NH2	1:E:291:GLU:HG3	2.24	0.52
1:B:236:LEU:O	1:B:237:GLN:HG2	2.10	0.52
1:C:295:LEU:HB2	1:C:305:ILE:HD13	1.92	0.52
1:C:292:PRO:O	1:C:296:ILE:HG13	2.10	0.51
1:D:338:GLN:O	1:D:342:ASN:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:388:PRO:HB2	1:E:66:THR:HG22	1.92	0.51
1:B:154:VAL:O	1:B:158:VAL:HG23	2.09	0.51
1:A:251:PHE:HB3	1:A:254:LEU:HB2	1.92	0.51
1:B:386:ASP:HB3	1:C:68:HIS:NE2	2.24	0.51
1:D:86:LYS:O	1:D:90:VAL:HG23	2.11	0.51
1:F:400:GLU:HB2	1:F:406:GLN:HE21	1.75	0.51
1:C:387:LEU:HA	1:C:390:MET:HE2	1.92	0.51
1:C:64:LEU:HD22	1:C:100:ARG:HD2	1.93	0.51
1:D:307:ARG:C	1:D:309:PRO:HD3	2.30	0.51
1:B:77:TYR:CE1	1:B:330:LYS:HD2	2.46	0.50
1:C:261:ARG:HD3	1:C:294:ASP:OD1	2.11	0.50
1:A:358:ILE:HD13	1:A:376:VAL:HG22	1.93	0.50
1:B:338:GLN:O	1:B:342:ASN:HB2	2.10	0.50
1:E:117:LEU:HD23	1:E:312:ALA:HB3	1.92	0.50
1:B:361:LYS:HB2	1:B:375:ILE:HD13	1.92	0.50
1:D:76:ASP:CB	1:D:330:LYS:HE3	2.34	0.50
1:E:91:ALA:HB2	1:E:310:VAL:HG11	1.92	0.50
1:C:125:LYS:HB2	2:C:500:SO4:O3	2.10	0.50
1:E:146:THR:O	1:E:149:THR:HG22	2.12	0.50
1:B:212:LEU:HD21	1:B:303:GLU:HG3	1.94	0.50
1:E:346:VAL:HG13	1:E:394:GLU:HA	1.93	0.50
1:E:385:TYR:OH	1:F:71:ARG:HD3	2.11	0.50
1:C:158:VAL:HG11	1:C:214:LEU:HB2	1.93	0.50
1:E:154:VAL:O	1:E:158:VAL:HG23	2.11	0.50
1:F:321:ALA:O	1:F:325:ILE:HG13	2.11	0.50
1:F:398:ILE:HB	1:F:400:GLU:HG2	1.93	0.50
1:B:396:VAL:HB	1:B:410:LEU:HB3	1.92	0.49
1:C:117:LEU:HD23	1:C:312:ALA:HB3	1.93	0.49
1:F:383:THR:O	1:F:387:LEU:HB2	2.11	0.49
1:A:154:VAL:O	1:A:158:VAL:HG23	2.12	0.49
1:A:209:GLN:O	1:A:212:LEU:HB3	2.12	0.49
1:C:81:GLN:HE22	1:C:316:GLU:H	1.59	0.49
1:C:377:GLU:OE2	1:D:310:VAL:HG22	2.11	0.49
1:E:212:LEU:CD1	1:E:307:ARG:HG3	2.42	0.49
1:F:158:VAL:HG11	1:F:214:LEU:HB2	1.94	0.49
1:F:295:LEU:HB2	1:F:305:ILE:HD13	1.94	0.49
1:A:146:THR:O	1:A:149:THR:HG22	2.13	0.49
1:A:360:LYS:HA	1:A:363:MET:CE	2.42	0.49
1:C:400:GLU:HB2	1:C:406:GLN:HE21	1.76	0.49
1:F:189:ILE:HD12	1:F:208:GLN:HG2	1.94	0.49
1:A:361:LYS:HB2	1:A:375:ILE:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LEU:O	1:B:154:VAL:HG21	2.11	0.49
1:A:369:ALA:HA	1:A:372:LEU:HG	1.94	0.49
1:B:307:ARG:O	1:B:309:PRO:HD3	2.12	0.49
1:D:282:SER:O	1:D:286:LEU:HD13	2.12	0.49
1:A:91:ALA:HB2	1:A:310:VAL:HG11	1.94	0.49
1:B:346:VAL:HG13	1:B:394:GLU:HA	1.95	0.49
1:C:240:THR:O	1:C:243:ILE:HG12	2.12	0.49
1:C:354:ALA:O	1:C:358:ILE:HG13	2.12	0.49
1:E:243:ILE:HD11	1:E:245:PHE:CZ	2.48	0.49
1:F:94:ASN:O	1:F:98:ARG:HG3	2.13	0.49
1:A:377:GLU:OE1	1:B:309:PRO:HB2	2.12	0.49
1:B:125:LYS:HB2	2:B:500:SO4:O3	2.11	0.49
1:B:338:GLN:HG2	1:B:348:LEU:HB3	1.95	0.49
1:D:148:LEU:O	1:D:154:VAL:HG21	2.11	0.49
1:E:357:ALA:HB1	1:E:403:ILE:CG1	2.35	0.49
1:F:163:GLN:O	1:F:167:GLN:HG3	2.12	0.49
1:F:292:PRO:O	1:F:296:ILE:HG13	2.13	0.48
1:A:217:GLY:HA3	1:A:241:SER:OG	2.12	0.48
1:C:94:ASN:O	1:C:98:ARG:HG3	2.12	0.48
1:C:189:ILE:O	1:C:204:GLY:HA3	2.13	0.48
1:F:117:LEU:HD23	1:F:312:ALA:HB3	1.94	0.48
1:C:383:THR:O	1:C:387:LEU:HB2	2.13	0.48
1:D:209:GLN:O	1:D:212:LEU:HB3	2.13	0.48
1:D:331:ASN:CG	1:E:109:GLU:HG3	2.34	0.48
1:F:240:THR:O	1:F:243:ILE:HG12	2.13	0.48
1:B:251:PHE:HB3	1:B:254:LEU:HB2	1.94	0.48
1:C:385:TYR:CD1	1:D:90:VAL:HG22	2.45	0.48
1:F:358:ILE:HD13	1:F:376:VAL:HG22	1.96	0.48
1:C:321:ALA:O	1:C:325:ILE:HG13	2.13	0.48
1:E:105:SER:HA	1:E:109:GLU:N	2.28	0.48
1:A:212:LEU:HD11	1:A:307:ARG:HG3	1.94	0.48
1:A:307:ARG:C	1:A:309:PRO:HD3	2.33	0.48
1:B:351:ARG:HD2	1:B:398:ILE:HG22	1.94	0.48
1:E:307:ARG:C	1:E:309:PRO:HD3	2.34	0.48
1:F:354:ALA:O	1:F:358:ILE:HG13	2.14	0.48
1:C:357:ALA:O	1:C:361:LYS:HG2	2.14	0.48
1:B:122:GLY:HA2	2:B:500:SO4:O4	2.14	0.47
1:D:76:ASP:O	1:D:329:PRO:HA	2.14	0.47
1:F:125:LYS:HB2	2:F:500:SO4:O3	2.13	0.47
1:E:182:TYR:HA	1:E:246:ILE:O	2.15	0.47
1:E:251:PHE:HB3	1:E:254:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ARG:NH1	1:A:375:ILE:HG12	2.30	0.47
1:B:146:THR:O	1:B:149:THR:HG22	2.14	0.47
1:D:388:PRO:HG2	1:E:67:PRO:HD3	1.96	0.47
1:E:148:LEU:O	1:E:154:VAL:HG21	2.14	0.47
1:A:354:ALA:O	1:A:358:ILE:HG13	2.14	0.47
1:B:287:LEU:O	1:B:313:THR:HG21	2.13	0.47
1:E:190:SER:HA	1:E:208:GLN:NE2	2.30	0.47
1:A:157:ASP:O	1:A:160:ASN:HB3	2.15	0.47
1:D:212:LEU:CD1	1:D:307:ARG:HG3	2.45	0.47
1:E:319:GLU:O	1:E:323:ILE:HG13	2.14	0.47
1:F:116:LEU:HD12	1:F:247:CYS:O	2.14	0.47
1:F:291:GLU:CG	1:F:292:PRO:HD2	2.45	0.47
1:E:354:ALA:O	1:E:358:ILE:HG13	2.13	0.47
1:B:91:ALA:HB2	1:B:310:VAL:HG11	1.97	0.47
1:E:321:ALA:O	1:E:325:ILE:HG13	2.15	0.47
1:F:356:ASP:O	1:F:360:LYS:HG3	2.15	0.47
1:B:307:ARG:C	1:B:309:PRO:HD3	2.35	0.47
1:B:328:GLU:HB2	1:B:329:PRO:HD3	1.97	0.47
1:E:286:LEU:N	1:E:286:LEU:CD1	2.78	0.47
1:E:396:VAL:HB	1:E:410:LEU:HB3	1.97	0.47
1:B:98:ARG:HD2	1:B:110:LEU:CB	2.46	0.46
1:B:282:SER:O	1:B:286:LEU:HD13	2.16	0.46
1:C:336:GLN:O	1:C:340:LEU:HD13	2.15	0.46
1:E:209:GLN:O	1:E:212:LEU:HB3	2.15	0.46
1:C:70:ILE:O	1:C:74:LEU:HG	2.16	0.46
1:C:185:GLU:HB3	1:C:188:LYS:HG3	1.98	0.46
1:C:356:ASP:O	1:C:360:LYS:HG3	2.16	0.46
1:A:149:THR:HA	1:A:207:VAL:HG21	1.98	0.46
1:A:373:ARG:HG2	1:B:309:PRO:HB3	1.97	0.46
1:B:200:ARG:HD2	1:B:200:ARG:N	2.31	0.46
1:B:212:LEU:HD21	1:B:303:GLU:CG	2.46	0.46
1:B:371:GLY:O	1:B:375:ILE:HG13	2.15	0.46
1:C:138:VAL:HG12	1:C:179:GLY:HA2	1.98	0.46
1:D:146:THR:O	1:D:149:THR:HG22	2.15	0.46
1:E:154:VAL:HA	1:E:157:ASP:HB3	1.97	0.46
1:F:336:GLN:O	1:F:340:LEU:HD13	2.14	0.46
1:C:398:ILE:HG22	1:C:399:ASP:N	2.30	0.46
1:D:307:ARG:O	1:D:309:PRO:HD3	2.16	0.46
1:D:365:ARG:NH1	1:D:375:ILE:HG12	2.31	0.46
1:F:261:ARG:HD3	1:F:294:ASP:OD1	2.16	0.46
1:C:149:THR:O	1:C:202:VAL:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:ILE:HG13	1:C:304:PHE:H	1.80	0.46
1:D:149:THR:HA	1:D:207:VAL:HG21	1.98	0.46
1:E:64:LEU:HA	1:E:65:PRO:HD3	1.78	0.46
1:C:82:GLU:OE2	1:C:86:LYS:HE3	2.15	0.46
1:D:371:GLY:O	1:D:375:ILE:HG13	2.15	0.46
1:A:396:VAL:HB	1:A:410:LEU:HB3	1.98	0.45
1:D:251:PHE:HB3	1:D:254:LEU:HB2	1.97	0.45
1:D:346:VAL:HG13	1:D:394:GLU:HA	1.99	0.45
1:A:112:LYS:CE	1:A:307:ARG:HE	2.29	0.45
1:A:243:ILE:HD11	1:A:245:PHE:CZ	2.51	0.45
1:B:381:LEU:HD11	1:C:86:LYS:HB3	1.98	0.45
1:C:341:PHE:CD1	1:C:348:LEU:HD22	2.51	0.45
1:D:361:LYS:HB2	1:D:375:ILE:HD13	1.98	0.45
1:A:346:VAL:HG13	1:A:394:GLU:HA	1.98	0.45
1:C:140:PHE:CE2	1:C:142:MET:HG3	2.51	0.45
1:A:200:ARG:HD2	1:A:200:ARG:N	2.31	0.45
1:B:371:GLY:HA2	1:C:291:GLU:OE1	2.17	0.45
1:B:392:ASP:HB3	1:B:413:TYR:CD2	2.52	0.45
1:D:369:ALA:HA	1:D:372:LEU:HG	1.98	0.45
1:E:307:ARG:O	1:E:309:PRO:HD3	2.16	0.45
1:B:403:ILE:HG13	1:B:404:ASP:N	2.30	0.45
1:D:154:VAL:HA	1:D:157:ASP:HB3	1.98	0.45
1:A:291:GLU:CD	1:F:365:ARG:HH12	2.20	0.45
1:C:81:GLN:HE22	1:C:315:ASN:H	1.64	0.45
1:F:122:GLY:HA2	1:F:325:ILE:HD11	1.98	0.45
1:F:301:ILE:HG13	1:F:304:PHE:H	1.82	0.45
1:D:200:ARG:HD2	1:D:200:ARG:N	2.31	0.45
1:E:327:LYS:HD2	1:E:355:LEU:HD13	1.98	0.45
1:F:317:LEU:HD13	1:F:368:GLY:HA2	1.99	0.45
1:A:251:PHE:HB3	1:A:254:LEU:CB	2.47	0.45
1:B:92:VAL:CG1	1:B:136:LEU:HD11	2.47	0.45
1:D:190:SER:HA	1:D:208:GLN:NE2	2.31	0.45
1:E:387:LEU:CB	1:E:388:PRO:HD3	2.43	0.45
1:A:357:ALA:O	1:A:361:LYS:HG2	2.16	0.45
1:D:212:LEU:HD21	1:D:303:GLU:CG	2.47	0.45
1:F:64:LEU:HD22	1:F:100:ARG:HD2	1.98	0.45
1:E:295:LEU:HB2	1:E:305:ILE:HD13	1.99	0.45
1:E:369:ALA:HA	1:E:372:LEU:HG	1.99	0.45
1:B:385:TYR:O	1:C:67:PRO:HB2	2.17	0.44
1:D:327:LYS:O	1:D:335:LYS:HE3	2.17	0.44
1:F:341:PHE:CD1	1:F:348:LEU:HD22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD21	1:A:303:GLU:HG3	1.98	0.44
1:A:330:LYS:HE2	1:A:330:LYS:HB3	1.80	0.44
1:E:200:ARG:N	1:E:200:ARG:HD2	2.32	0.44
1:E:303:GLU:OE1	1:E:303:GLU:HA	2.17	0.44
1:E:371:GLY:O	1:E:375:ILE:HG13	2.18	0.44
1:A:264:THR:HG23	1:A:264:THR:O	2.16	0.44
1:E:317:LEU:HD13	1:E:325:ILE:CD1	2.48	0.44
1:D:357:ALA:O	1:D:361:LYS:HG2	2.18	0.44
1:E:174:GLN:HG3	1:E:175:LYS:N	2.32	0.44
1:E:212:LEU:HD21	1:E:303:GLU:HG3	1.99	0.44
1:E:217:GLY:HA3	1:E:241:SER:HG	1.82	0.44
1:F:243:ILE:HD11	1:F:245:PHE:CZ	2.53	0.44
1:D:331:ASN:OD1	1:E:109:GLU:HG3	2.17	0.44
1:A:76:ASP:HB3	1:A:330:LYS:HE3	1.99	0.44
1:A:136:LEU:O	1:A:138:VAL:HG23	2.18	0.44
1:E:282:SER:O	1:E:286:LEU:HD13	2.17	0.44
1:E:328:GLU:HB2	1:E:329:PRO:HD3	2.00	0.44
1:E:388:PRO:HB3	1:F:93:TYR:CZ	2.52	0.44
1:F:189:ILE:O	1:F:204:GLY:HA3	2.17	0.44
1:A:212:LEU:HD21	1:A:303:GLU:CG	2.47	0.44
1:B:160:ASN:HA	1:B:163:GLN:HG2	1.99	0.44
1:E:280:LYS:CB	1:E:286:LEU:HD11	2.48	0.44
1:F:208:GLN:O	1:F:212:LEU:HB2	2.18	0.44
1:B:157:ASP:O	1:B:160:ASN:HB3	2.17	0.44
1:C:347:ASP:O	1:C:394:GLU:HB2	2.18	0.44
1:F:307:ARG:C	1:F:309:PRO:HD3	2.38	0.44
1:C:291:GLU:CG	1:C:292:PRO:HD2	2.47	0.43
1:D:388:PRO:HG2	1:E:67:PRO:CD	2.48	0.43
1:E:136:LEU:O	1:E:138:VAL:HG23	2.18	0.43
1:A:343:LEU:HD13	1:B:97:LYS:HE3	2.00	0.43
1:D:212:LEU:HD21	1:D:303:GLU:HG3	1.99	0.43
1:D:338:GLN:HG2	1:D:348:LEU:HB3	1.99	0.43
1:B:119:GLY:O	1:B:250:ALA:HA	2.18	0.43
1:B:136:LEU:O	1:B:138:VAL:HG23	2.18	0.43
1:E:212:LEU:HD21	1:E:303:GLU:CG	2.48	0.43
1:C:318:SER:H	1:C:321:ALA:HB3	1.82	0.43
1:E:357:ALA:O	1:E:361:LYS:HG2	2.18	0.43
1:A:403:ILE:HG13	1:A:404:ASP:N	2.31	0.43
1:B:208:GLN:O	1:B:212:LEU:HB2	2.18	0.43
1:B:243:ILE:HD11	1:B:245:PHE:CZ	2.53	0.43
1:D:328:GLU:HB2	1:D:329:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:ASP:O	1:E:160:ASN:HB3	2.18	0.43
1:E:259:SER:OG	1:E:286:LEU:HD23	2.19	0.43
1:A:371:GLY:O	1:A:375:ILE:HG13	2.18	0.43
1:B:154:VAL:HA	1:B:157:ASP:HB3	2.01	0.43
1:F:70:ILE:O	1:F:74:LEU:HG	2.18	0.43
1:A:303:GLU:OE1	1:A:303:GLU:HA	2.19	0.43
1:A:307:ARG:O	1:A:309:PRO:HD3	2.19	0.43
1:B:303:GLU:HA	1:B:303:GLU:OE1	2.19	0.43
1:E:133:ALA:CB	1:E:140:PHE:HB2	2.48	0.43
1:E:160:ASN:HA	1:E:163:GLN:HG2	2.01	0.43
1:A:64:LEU:HA	1:A:65:PRO:HD3	1.78	0.43
1:A:327:LYS:HD2	1:A:355:LEU:HD13	2.00	0.43
1:C:116:LEU:HD12	1:C:247:CYS:O	2.19	0.43
1:C:353:GLU:OE2	1:C:398:ILE:HG23	2.19	0.43
1:D:140:PHE:CE2	1:D:142:MET:HG3	2.53	0.43
1:D:327:LYS:HD2	1:D:355:LEU:HD13	2.01	0.43
1:E:347:ASP:O	1:E:394:GLU:HB2	2.19	0.43
1:F:317:LEU:CD1	1:F:368:GLY:HA2	2.49	0.43
1:E:212:LEU:HD11	1:E:307:ARG:HG3	2.00	0.43
1:E:392:ASP:HB3	1:E:413:TYR:CD1	2.53	0.43
1:B:251:PHE:HB3	1:B:254:LEU:CB	2.49	0.42
1:C:361:LYS:O	1:C:365:ARG:HG3	2.19	0.42
1:E:216:GLU:OE1	1:E:307:ARG:HD2	2.19	0.42
1:A:90:VAL:HG12	1:A:94:ASN:ND2	2.33	0.42
1:A:165:LEU:O	1:A:169:CYS:HB2	2.18	0.42
1:C:361:LYS:HE3	1:C:365:ARG:HH21	1.84	0.42
1:D:160:ASN:HA	1:D:163:GLN:HG2	2.01	0.42
1:D:212:LEU:HD11	1:D:307:ARG:HG3	2.01	0.42
1:F:114:ASN:HB2	1:F:307:ARG:O	2.19	0.42
1:A:347:ASP:O	1:A:394:GLU:HB2	2.19	0.42
1:C:133:ALA:CB	1:C:140:PHE:HB2	2.49	0.42
1:F:296:ILE:HA	1:F:300:LEU:O	2.20	0.42
1:A:166:LEU:HA	1:A:169:CYS:HB3	2.01	0.42
1:B:64:LEU:HA	1:B:65:PRO:HD3	1.79	0.42
1:D:295:LEU:HB2	1:D:305:ILE:HD13	2.01	0.42
1:A:327:LYS:O	1:A:335:LYS:HE3	2.20	0.42
1:A:295:LEU:HB2	1:A:305:ILE:HD13	2.01	0.42
1:C:189:ILE:HD12	1:C:208:GLN:HG2	2.02	0.42
1:C:329:PRO:C	1:C:331:ASN:H	2.22	0.42
1:F:149:THR:O	1:F:202:VAL:HB	2.19	0.42
1:A:160:ASN:HA	1:A:163:GLN:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:PHE:CD1	1:B:348:LEU:HD22	2.54	0.42
1:A:386:ASP:O	1:A:390:MET:HG3	2.19	0.42
1:B:209:GLN:O	1:B:212:LEU:HB3	2.19	0.42
1:D:98:ARG:HD2	1:D:110:LEU:CB	2.50	0.42
1:D:358:ILE:HD13	1:D:376:VAL:HG22	2.02	0.42
1:A:363:MET:HE2	1:A:363:MET:HB2	1.86	0.42
1:B:149:THR:HA	1:B:207:VAL:HG21	2.02	0.42
1:D:347:ASP:O	1:D:394:GLU:HB2	2.19	0.42
1:E:388:PRO:HG2	1:F:67:PRO:HD3	2.01	0.42
1:A:128:LEU:O	1:A:132:LEU:HG	2.19	0.42
1:D:292:PRO:O	1:D:296:ILE:HG12	2.19	0.42
1:C:114:ASN:HB2	1:C:307:ARG:O	2.19	0.41
1:D:321:ALA:O	1:D:325:ILE:HG13	2.20	0.41
1:E:386:ASP:O	1:E:390:MET:HG3	2.20	0.41
1:A:78:VAL:HG21	1:A:128:LEU:CD2	2.48	0.41
1:A:216:GLU:OE1	1:A:307:ARG:HD2	2.20	0.41
1:E:331:ASN:HB3	1:E:336:GLN:HE21	1.84	0.41
1:E:338:GLN:HG2	1:E:348:LEU:HB3	2.02	0.41
1:A:190:SER:HA	1:A:208:GLN:NE2	2.35	0.41
1:A:154:VAL:HA	1:A:157:ASP:HB3	2.02	0.41
1:B:327:LYS:O	1:B:335:LYS:HE3	2.20	0.41
1:C:208:GLN:O	1:C:212:LEU:HB2	2.20	0.41
1:E:149:THR:HA	1:E:207:VAL:HG21	2.01	0.41
1:F:161:ILE:HD11	1:F:214:LEU:CD2	2.51	0.41
1:C:141:THR:HG22	1:C:165:LEU:HD13	2.02	0.41
1:F:133:ALA:CB	1:F:140:PHE:HB2	2.51	0.41
1:B:388:PRO:HG2	1:C:67:PRO:CD	2.51	0.41
1:C:95:HIS:CD2	1:C:244:LEU:HD13	2.56	0.41
1:A:140:PHE:CE2	1:A:142:MET:HG3	2.56	0.41
1:B:354:ALA:O	1:B:358:ILE:HG13	2.21	0.41
1:B:386:ASP:O	1:B:390:MET:HG3	2.20	0.41
1:D:403:ILE:HG13	1:D:404:ASP:N	2.34	0.41
1:F:347:ASP:O	1:F:394:GLU:HB2	2.21	0.41
1:F:395:LYS:HA	1:F:410:LEU:O	2.21	0.41
1:A:176:ALA:O	1:A:243:ILE:HG22	2.20	0.41
1:A:182:TYR:HA	1:A:246:ILE:O	2.20	0.41
1:B:347:ASP:O	1:B:394:GLU:HB2	2.21	0.41
1:B:408:GLU:HB3	1:B:409:PRO:HD2	2.03	0.41
1:C:211:LEU:O	1:C:214:LEU:HB3	2.21	0.41
1:C:307:ARG:C	1:C:309:PRO:HD3	2.41	0.41
1:D:79:ILE:HD11	1:D:329:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:ASP:O	1:D:160:ASN:HB3	2.21	0.41
1:D:251:PHE:HB3	1:D:254:LEU:CB	2.51	0.41
1:D:385:TYR:OH	1:E:71:ARG:HD3	2.21	0.41
1:E:344:GLU:OE2	1:F:93:TYR:HE2	2.04	0.41
1:F:112:LYS:O	1:F:309:PRO:HG2	2.21	0.41
1:F:399:ASP:O	1:F:403:ILE:HG22	2.21	0.41
1:B:292:PRO:O	1:B:296:ILE:HG12	2.21	0.41
1:B:369:ALA:HA	1:B:372:LEU:HG	2.03	0.41
1:D:303:GLU:HA	1:D:303:GLU:OE1	2.20	0.41
1:D:386:ASP:O	1:D:390:MET:HG3	2.20	0.41
1:E:251:PHE:HB3	1:E:254:LEU:CB	2.51	0.41
1:E:292:PRO:O	1:E:296:ILE:HG12	2.21	0.41
1:F:185:GLU:HB3	1:F:188:LYS:HG3	2.02	0.41
1:A:86:LYS:O	1:A:90:VAL:HG23	2.21	0.40
1:C:138:VAL:HG13	1:C:139:PRO:HD2	2.03	0.40
1:D:243:ILE:HD11	1:D:245:PHE:CZ	2.56	0.40
1:E:119:GLY:O	1:E:250:ALA:HA	2.21	0.40
1:F:141:THR:HG22	1:F:165:LEU:HD13	2.04	0.40
1:A:86:LYS:HG3	1:F:385:TYR:CZ	2.55	0.40
1:B:92:VAL:HG11	1:B:136:LEU:HD11	2.02	0.40
1:D:128:LEU:O	1:D:132:LEU:HG	2.21	0.40
1:F:190:SER:HB3	1:F:300:LEU:HD12	2.03	0.40
1:B:392:ASP:HB3	1:B:413:TYR:CE2	2.55	0.40
1:C:329:PRO:C	1:C:331:ASN:N	2.73	0.40
1:F:367:THR:HB	1:F:371:GLY:HA3	2.04	0.40
1:B:182:TYR:HA	1:B:246:ILE:O	2.22	0.40
1:B:357:ALA:O	1:B:361:LYS:HG2	2.21	0.40
1:E:327:LYS:O	1:E:335:LYS:HE3	2.21	0.40
1:E:296:ILE:CD1	1:E:305:ILE:HD12	2.52	0.40
1:F:195:ASN:HA	1:F:196:PRO:HD2	1.93	0.40
1:F:199:THR:HG22	1:F:201:ASP:N	2.36	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	299/363 (82%)	286 (96%)	13 (4%)	0	100	100
1	B	295/363 (81%)	281 (95%)	14 (5%)	0	100	100
1	C	288/363 (79%)	274 (95%)	13 (4%)	1 (0%)	41	76
1	D	298/363 (82%)	285 (96%)	13 (4%)	0	100	100
1	E	303/363 (84%)	291 (96%)	12 (4%)	0	100	100
1	F	295/363 (81%)	281 (95%)	13 (4%)	1 (0%)	41	76
All	All	1778/2178 (82%)	1698 (96%)	78 (4%)	2 (0%)	51	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	103	ASP
1	C	103	ASP

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	243/299 (81%)	243 (100%)	0	100	100
1	B	241/299 (81%)	241 (100%)	0	100	100
1	C	242/299 (81%)	242 (100%)	0	100	100
1	D	241/299 (81%)	241 (100%)	0	100	100
1	E	244/299 (82%)	244 (100%)	0	100	100
1	F	247/299 (83%)	247 (100%)	0	100	100
All	All	1458/1794 (81%)	1458 (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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	B	83	GLN
1	C	81	GLN
1	C	101	ASN
1	C	406	GLN
1	E	83	GLN
1	F	81	GLN
1	F	101	ASN
1	F	406	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	E	500	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	A	500	-	4,4,4	0.15	0	6,6,6	0.04	0
2	SO4	C	500	-	4,4,4	0.15	0	6,6,6	0.04	0
2	SO4	F	500	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	500	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	D	500	-	4,4,4	0.15	0	6,6,6	0.05	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.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	500	SO4	1	0
2	A	500	SO4	1	0
2	C	500	SO4	1	0
2	F	500	SO4	1	0
2	B	500	SO4	2	0
2	D	500	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	311/363 (85%)	0.90	41 (13%)	3	6	221, 311, 448, 562	0
1	B	307/363 (84%)	0.71	32 (10%)	6	8	188, 302, 448, 502	0
1	C	298/363 (82%)	0.87	31 (10%)	6	8	205, 303, 437, 529	0
1	D	310/363 (85%)	0.57	29 (9%)	8	10	217, 309, 429, 492	0
1	E	315/363 (86%)	0.65	30 (9%)	8	10	254, 330, 398, 461	0
1	F	305/363 (84%)	0.54	22 (7%)	15	15	201, 298, 486, 605	0
All	All	1846/2178 (84%)	0.71	185 (10%)	7	9	188, 310, 444, 605	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	GLY	13.0
1	B	200	ARG	9.6
1	A	266	SER	8.3
1	F	195	ASN	8.3
1	F	197	SER	7.7
1	A	264	THR	7.6
1	C	103	ASP	7.0
1	A	263	GLU	6.9
1	B	266	SER	6.5
1	D	266	SER	6.3
1	B	203	SER	6.0
1	A	149	THR	5.9
1	C	101	ASN	5.9
1	C	191	ARG	5.5
1	B	63	ALA	5.4
1	D	195	ASN	5.4
1	A	203	SER	5.3
1	C	102	GLY	5.2
1	C	100	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	235	PHE	4.8
1	F	153	TYR	4.8
1	E	203	SER	4.6
1	B	149	THR	4.6
1	A	344	GLU	4.6
1	C	154	VAL	4.6
1	D	196	PRO	4.6
1	C	162	ILE	4.6
1	F	196	PRO	4.5
1	C	104	THR	4.5
1	C	150	GLU	4.4
1	D	392	ASP	4.4
1	D	315	ASN	4.3
1	D	193	SER	4.3
1	A	104	THR	4.3
1	A	105	SER	4.2
1	D	264	THR	4.2
1	C	153	TYR	4.2
1	E	317	LEU	4.2
1	B	265	GLY	4.1
1	D	237	GLN	4.1
1	A	390	MET	4.1
1	E	350	PHE	4.1
1	B	218	THR	4.1
1	A	392	ASP	4.1
1	E	149	THR	4.0
1	C	282	SER	3.9
1	C	149	THR	3.9
1	E	79	ILE	3.9
1	B	204	GLY	3.9
1	B	201	ASP	3.8
1	A	200	ARG	3.7
1	A	351	ARG	3.7
1	E	265	GLY	3.7
1	C	161	ILE	3.7
1	C	158	VAL	3.6
1	A	238	VAL	3.6
1	A	388	PRO	3.6
1	E	264	THR	3.5
1	C	237	GLN	3.5
1	C	159	GLU	3.5
1	D	64	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	237	GLN	3.4
1	D	236	LEU	3.4
1	E	266	SER	3.4
1	A	317	LEU	3.4
1	E	64	LEU	3.4
1	E	200	ARG	3.4
1	B	102	GLY	3.3
1	D	238	VAL	3.3
1	E	349	GLU	3.2
1	B	254	LEU	3.2
1	F	368	GLY	3.2
1	D	394	GLU	3.2
1	F	198	ILE	3.2
1	C	236	LEU	3.2
1	F	103	ASP	3.2
1	B	103	ASP	3.1
1	B	202	VAL	3.1
1	C	350	PHE	3.1
1	A	411	LEU	3.0
1	E	394	GLU	3.0
1	A	261	ARG	3.0
1	D	411	LEU	3.0
1	E	78	VAL	3.0
1	E	238	VAL	3.0
1	D	235	PHE	3.0
1	E	80	GLY	3.0
1	F	369	ALA	3.0
1	F	207	VAL	2.9
1	D	282	SER	2.9
1	F	154	VAL	2.9
1	A	410	LEU	2.9
1	A	103	ASP	2.9
1	C	96	TYR	2.9
1	D	194	ASP	2.9
1	A	204	GLY	2.9
1	D	265	GLY	2.9
1	A	207	VAL	2.8
1	B	104	THR	2.8
1	F	171	TYR	2.8
1	A	64	LEU	2.8
1	B	396	VAL	2.8
1	E	65	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	119	GLY	2.8
1	A	178	ARG	2.8
1	E	251	PHE	2.7
1	A	350	PHE	2.7
1	B	264	THR	2.7
1	D	344	GLU	2.7
1	E	279	ASP	2.7
1	B	97	LYS	2.7
1	D	63	ALA	2.6
1	C	252	ALA	2.6
1	E	334	THR	2.6
1	A	387	LEU	2.6
1	C	238	VAL	2.6
1	C	136	LEU	2.6
1	A	237	GLN	2.6
1	B	101	ASN	2.6
1	B	258	ILE	2.6
1	A	289	GLN	2.5
1	B	64	LEU	2.5
1	E	152	GLY	2.5
1	A	139	PRO	2.5
1	A	316	GLU	2.5
1	F	203	SER	2.5
1	B	289	GLN	2.4
1	A	409	PRO	2.4
1	E	153	TYR	2.4
1	C	284	GLY	2.4
1	B	239	ASP	2.4
1	C	170	ASP	2.4
1	F	152	GLY	2.4
1	A	345	GLY	2.4
1	B	112	LYS	2.4
1	D	395	LYS	2.4
1	E	100	ARG	2.4
1	E	173	VAL	2.4
1	B	255	ASP	2.3
1	E	207	VAL	2.3
1	D	348	LEU	2.3
1	D	192	LYS	2.3
1	C	327	LYS	2.3
1	B	350	PHE	2.3
1	C	155	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	350	PHE	2.3
1	A	327	LYS	2.3
1	A	408	GLU	2.3
1	F	370	ARG	2.3
1	E	254	LEU	2.3
1	E	236	LEU	2.3
1	E	187	ASP	2.2
1	D	176	ALA	2.2
1	F	163	GLN	2.2
1	B	287	LEU	2.2
1	B	147	THR	2.2
1	F	112	LYS	2.2
1	D	203	SER	2.2
1	C	315	ASN	2.2
1	E	356	ASP	2.2
1	F	64	LEU	2.2
1	D	410	LEU	2.2
1	C	65	PRO	2.1
1	F	309	PRO	2.1
1	E	235	PHE	2.1
1	B	368	GLY	2.1
1	A	307	ARG	2.1
1	F	307	ARG	2.1
1	A	326	LEU	2.1
1	B	286	LEU	2.1
1	F	237	GLN	2.1
1	C	316	GLU	2.1
1	D	93	TYR	2.1
1	A	141	THR	2.1
1	D	409	PRO	2.1
1	C	97	LYS	2.1
1	A	180	ILE	2.0
1	A	368	GLY	2.0
1	F	238	VAL	2.0
1	A	175	LYS	2.0
1	B	189	ILE	2.0
1	B	236	LEU	2.0
1	A	297	LYS	2.0
1	C	156	GLU	2.0
1	F	165	LEU	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	500	5/5	0.82	0.44	202,202,210,220	0
2	SO4	E	500	5/5	0.89	0.25	203,204,209,215	0
2	SO4	C	500	5/5	0.91	0.28	200,203,210,217	0
2	SO4	D	500	5/5	0.95	0.37	191,193,199,205	0
2	SO4	A	500	5/5	0.95	0.26	190,191,201,210	0
2	SO4	F	500	5/5	0.95	0.22	200,202,208,215	0

6.5 Other polymers (i)

There are no such residues in this entry.