Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:52 PM GMT

PDB ID	:	1YRL
Title	:	Escherichia coli ketol-acid reductoisomerase
Authors	:	Tyagi, R.; Duquerroy, S.; Navaza, J.; Guddat, L.W.; Duggleby, R.G.
Deposited on	:	2005-02-04
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

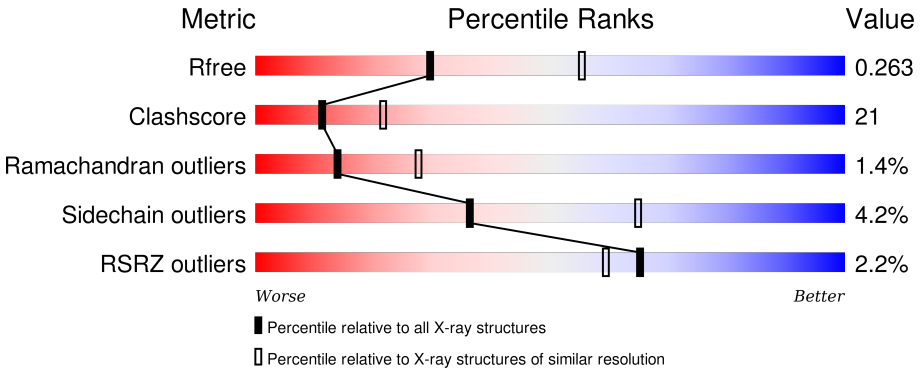
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	491	68% 29%
1	B	491	3% 50% 36% 12%
1	C	491	3% 60% 36%
1	D	491	3% 56% 36%

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	4126	-	X	-	-

2 Entry composition

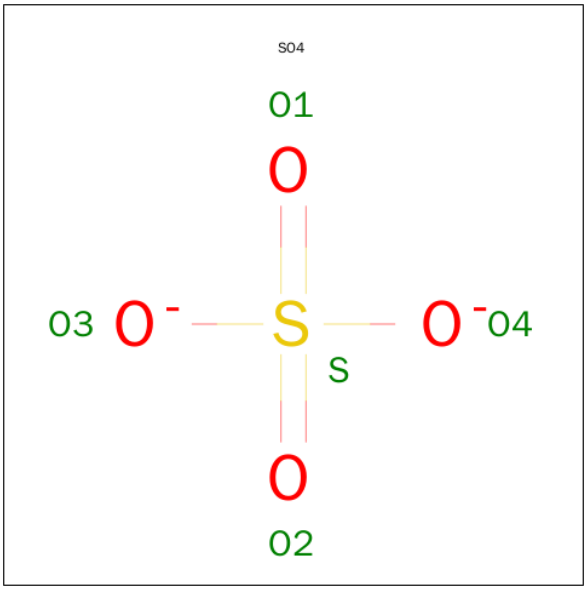
There are 3 unique types of molecules in this entry. The entry contains 14904 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ketol-acid reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3763	2379	638	720	26			
1	B	431	Total	C	N	O	S	0	0	0
			3320	2101	558	637	24			
1	C	487	Total	C	N	O	S	0	0	0
			3749	2370	633	720	26			
1	D	470	Total	C	N	O	S	0	0	0
			3611	2289	602	695	25			

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



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

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

- Molecule 3 is water.

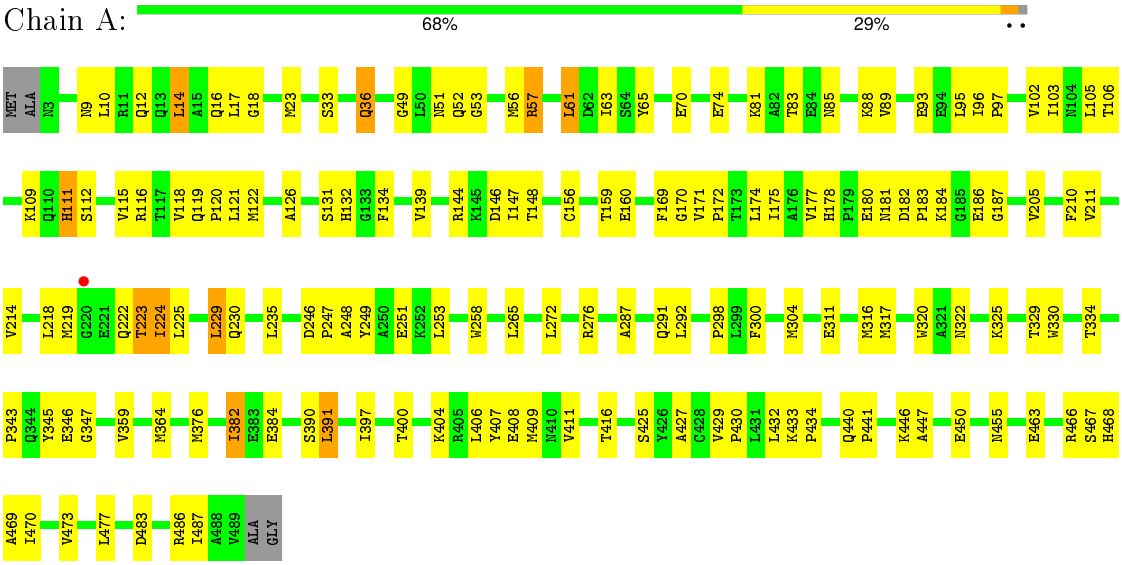
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	185	Total O 185 185	0	0
3	B	36	Total O 36 36	0	0
3	C	99	Total O 99 99	0	0
3	D	96	Total O 96 96	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

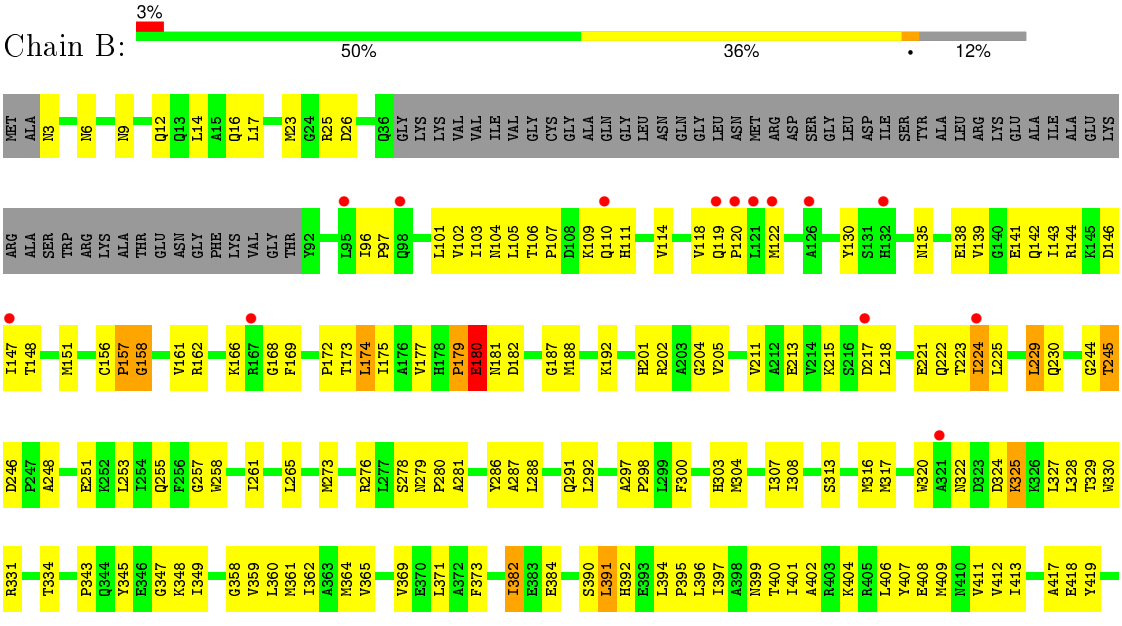
- Molecule 1: Ketol-acid reductoisomerase

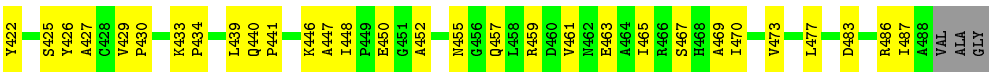
Chain A:



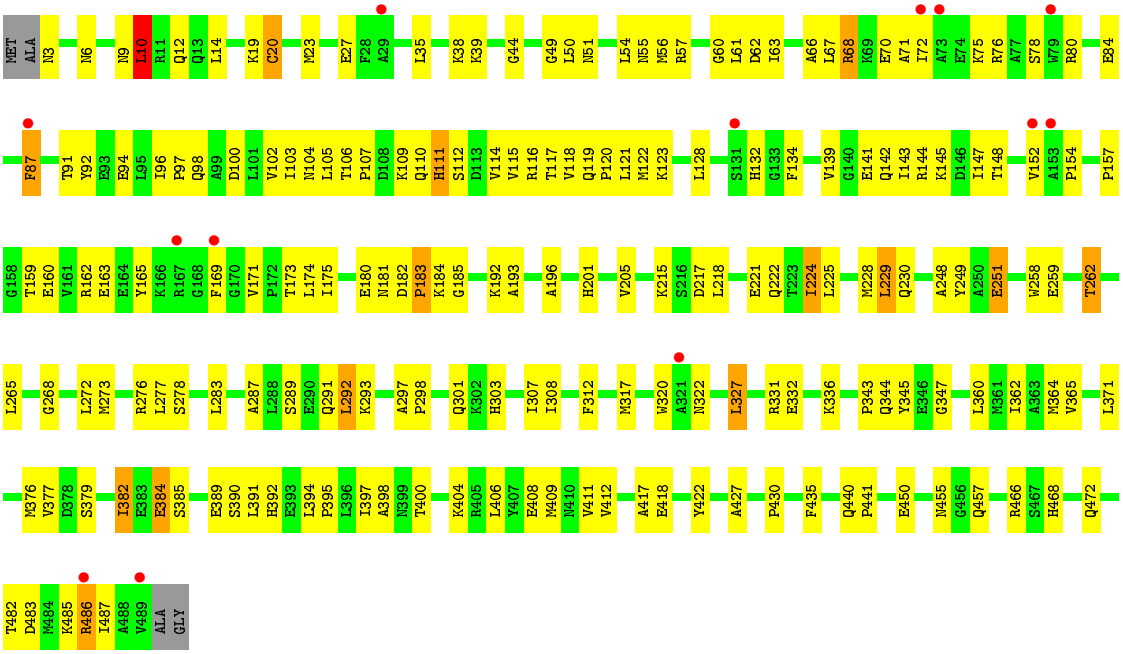
- Molecule 1: Ketol-acid reductoisomerase

Chain B:

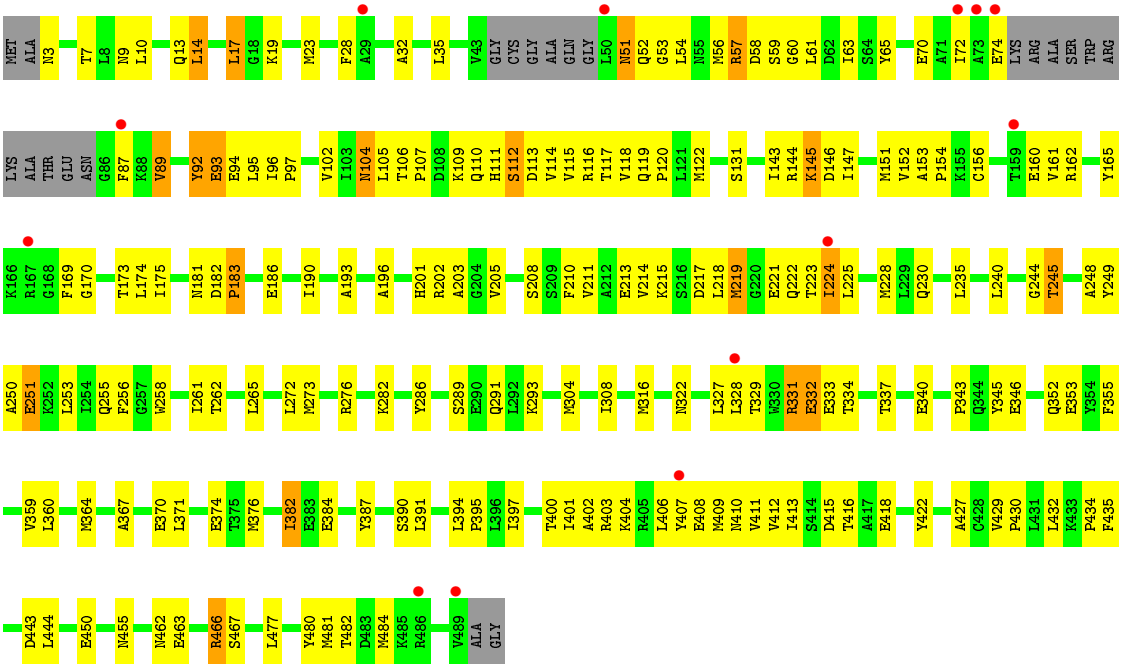




• Molecule 1: Ketol-acid reductoisomerase



• Molecule 1: Ketol-acid reductoisomerase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	226.88Å 226.88Å 118.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.48 – 2.60 32.48 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (32.48-2.60) 99.9 (32.48-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.15 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.266 0.221 , 0.263	Depositor DCC
R_{free} test set	10702 reflections (10.02%)	DCC
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.8	EDS
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Outliers	0 of 106782 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14904	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.41	0/3829	0.60	0/5164
1	B	0.36	0/3380	0.53	0/4564
1	C	0.37	0/3815	0.55	0/5149
1	D	0.37	0/3673	0.56	0/4957
All	All	0.38	0/14697	0.56	0/19834

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

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	3763	0	3751	136	0
1	B	3320	0	3276	147	0
1	C	3749	0	3718	177	0
1	D	3611	0	3568	155	0
2	A	20	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	15	0	0	0	0
3	A	185	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	36	0	0	2	0
3	C	99	0	0	4	0
3	D	96	0	0	4	0
All	All	14904	0	14313	594	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 21.

All (594) 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:382:ILE:H	1:B:382:ILE:HD12	1.13	1.08
1:C:382:ILE:H	1:C:382:ILE:HD12	1.23	1.04
1:D:382:ILE:H	1:D:382:ILE:HD12	1.29	0.98
1:A:455:ASN:HD21	1:C:276:ARG:HH11	1.17	0.93
1:A:330:TRP:O	1:A:334:THR:HG22	1.68	0.92
1:D:154:PRO:HA	1:D:173:THR:HG22	1.50	0.92
1:D:144:ARG:HD2	1:D:146:ASP:OD1	1.70	0.90
1:B:404:LYS:HB2	1:B:408:GLU:HB2	1.56	0.88
1:C:400:THR:HG21	1:C:409:MET:HA	1.60	0.82
1:C:154:PRO:HA	1:C:173:THR:HG22	1.61	0.81
1:A:382:ILE:HD12	1:A:382:ILE:H	1.46	0.81
1:C:258:TRP:O	1:C:262:THR:HB	1.79	0.80
1:A:223:THR:HG22	1:A:224:ILE:N	1.97	0.80
1:C:404:LYS:HB2	1:C:408:GLU:HB2	1.63	0.80
1:C:96:ILE:HD12	1:C:121:LEU:HD12	1.65	0.79
1:D:360:LEU:O	1:D:364:MET:HG3	1.82	0.79
1:A:23:MET:CE	1:A:205:VAL:HG12	2.12	0.79
1:A:112:SER:O	1:A:116:ARG:HG2	1.83	0.78
1:C:96:ILE:HD13	1:C:118:VAL:HG13	1.65	0.78
1:B:360:LEU:O	1:B:364:MET:HG3	1.84	0.76
1:A:404:LYS:HB2	1:A:408:GLU:HB2	1.65	0.76
1:B:455:ASN:HD21	1:D:276:ARG:HH11	1.32	0.76
1:B:265:LEU:HB2	1:B:273:MET:HE2	1.67	0.75
1:C:382:ILE:N	1:C:382:ILE:HD12	2.01	0.74
1:A:96:ILE:N	1:A:97:PRO:HD2	2.02	0.74
1:D:404:LYS:HB2	1:D:408:GLU:HB2	1.70	0.74
1:B:162:ARG:HE	1:B:166:LYS:HE3	1.53	0.73
1:B:230:GLN:HG3	1:B:406:LEU:HD13	1.71	0.73
1:A:276:ARG:HH11	1:C:455:ASN:HD21	1.35	0.73
1:C:486:ARG:HH21	1:C:486:ARG:HB2	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:ILE:N	1:D:97:PRO:HD2	2.03	0.72
1:B:404:LYS:CB	1:B:408:GLU:HB2	2.20	0.72
1:A:298:PRO:HG2	3:A:4142:HOH:O	1.89	0.72
1:A:218:LEU:O	1:A:222:GLN:HG2	1.89	0.71
1:B:418:GLU:HG2	1:B:422:TYR:CE1	2.25	0.71
1:C:60:GLY:C	1:C:61:LEU:HD12	2.10	0.71
1:D:400:THR:HG21	1:D:409:MET:HA	1.71	0.71
1:B:450:GLU:HG2	1:D:450:GLU:HG2	1.71	0.71
1:D:224:ILE:HA	1:D:228:MET:HB2	1.74	0.70
1:D:154:PRO:CA	1:D:173:THR:HG22	2.22	0.70
1:B:407:TYR:O	1:B:411:VAL:HG23	1.90	0.70
1:B:130:TYR:HE2	1:B:135:ASN:HB3	1.55	0.70
1:A:400:THR:HG21	1:A:409:MET:HA	1.74	0.70
1:A:224:ILE:HD13	1:A:224:ILE:O	1.91	0.69
1:A:9:ASN:OD1	1:A:12:GLN:HG3	1.91	0.69
1:A:106:THR:O	1:A:111:HIS:HE1	1.75	0.69
1:A:404:LYS:CB	1:A:408:GLU:HB2	2.22	0.69
1:B:429:VAL:HB	1:B:430:PRO:HD3	1.74	0.69
1:A:249:TYR:HA	1:A:345:TYR:HB2	1.75	0.69
1:D:382:ILE:HD12	1:D:382:ILE:N	2.05	0.68
1:C:360:LEU:O	1:C:364:MET:HG3	1.93	0.68
1:B:457:GLN:O	1:B:461:VAL:HG23	1.94	0.68
1:A:139:VAL:HG22	1:A:317:MET:CE	2.24	0.68
1:D:10:LEU:CD2	1:D:14:LEU:HD22	2.24	0.67
1:D:225:LEU:HB3	1:D:397:ILE:HD12	1.76	0.67
1:A:469:ALA:O	1:A:473:VAL:HG23	1.94	0.67
1:B:287:ALA:O	1:B:291:GLN:HG3	1.95	0.67
1:D:409:MET:O	1:D:413:ILE:HG12	1.95	0.67
1:C:278:SER:HB2	1:C:450:GLU:HG3	1.76	0.67
1:A:103:ILE:HG22	1:A:105:LEU:HG	1.77	0.67
1:B:119:GLN:HB2	1:B:120:PRO:HD3	1.77	0.67
1:C:382:ILE:HD13	1:C:385:SER:HB2	1.77	0.67
1:D:282:LYS:NZ	1:D:462:ASN:HD21	1.93	0.67
1:D:434:PRO:HG2	3:D:4164:HOH:O	1.94	0.67
1:A:18:GLY:HA2	1:A:382:ILE:HG13	1.76	0.66
1:B:348:LYS:HD3	1:B:349:ILE:H	1.60	0.66
1:C:215:LYS:HE3	1:C:307:ILE:O	1.95	0.66
1:B:401:ILE:HD11	1:B:409:MET:CE	2.25	0.66
1:A:219:MET:O	1:A:223:THR:HB	1.96	0.65
1:C:102:VAL:HG11	1:C:118:VAL:HG11	1.75	0.65
1:A:119:GLN:HB2	1:A:120:PRO:HD3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:GLN:HB2	1:D:120:PRO:HD3	1.78	0.65
1:C:9:ASN:OD1	1:C:12:GLN:HG3	1.95	0.65
1:D:114:VAL:O	1:D:118:VAL:HG23	1.96	0.65
1:C:119:GLN:HB2	1:C:120:PRO:HD3	1.78	0.65
1:A:178:HIS:HD2	3:A:4193:HOH:O	1.80	0.64
1:D:429:VAL:HB	1:D:430:PRO:HD3	1.77	0.64
1:B:452:ALA:HB2	1:D:352:GLN:HB2	1.78	0.64
1:A:382:ILE:HD12	1:A:382:ILE:N	2.10	0.64
1:D:218:LEU:O	1:D:222:GLN:HG2	1.98	0.64
1:D:258:TRP:HH2	1:D:364:MET:HE3	1.62	0.64
1:C:54:LEU:HB3	1:C:162:ARG:NH1	2.13	0.64
1:A:57:ARG:CG	1:A:57:ARG:HH21	2.10	0.64
1:D:463:GLU:HG2	3:D:4170:HOH:O	1.98	0.64
1:D:265:LEU:HG	1:D:391:LEU:HD11	1.80	0.63
1:A:455:ASN:ND2	1:C:276:ARG:HH11	1.92	0.63
1:B:114:VAL:O	1:B:118:VAL:HG23	1.99	0.63
1:D:282:LYS:HZ2	1:D:462:ASN:HD21	1.45	0.63
1:B:382:ILE:H	1:B:382:ILE:CD1	1.89	0.63
1:B:276:ARG:HH11	1:D:455:ASN:HD21	1.46	0.63
1:D:94:GLU:HG2	1:D:94:GLU:O	1.99	0.63
1:C:23:MET:HE3	1:C:205:VAL:HG12	1.80	0.63
1:C:262:THR:HG21	1:C:398:ALA:HB3	1.81	0.62
1:D:224:ILE:O	1:D:224:ILE:HD13	1.99	0.62
1:A:345:TYR:CZ	1:A:347:GLY:HA3	2.34	0.62
1:A:23:MET:HE1	1:A:205:VAL:CG1	2.28	0.62
1:C:482:THR:HA	1:C:485:LYS:HE2	1.81	0.62
1:A:23:MET:HE1	1:A:205:VAL:HG12	1.80	0.62
1:A:14:LEU:HD11	1:D:14:LEU:HD21	1.82	0.62
1:B:258:TRP:HB2	3:B:4150:HOH:O	1.98	0.62
1:D:382:ILE:CD1	1:D:382:ILE:H	1.99	0.62
1:A:93:GLU:H	1:A:93:GLU:CD	2.03	0.62
1:A:223:THR:HG23	1:A:300:PHE:CE2	2.34	0.62
1:C:400:THR:CG2	1:C:409:MET:HA	2.29	0.61
1:B:142:GLN:C	1:B:143:ILE:HD12	2.21	0.61
1:A:144:ARG:HD2	1:A:146:ASP:OD1	2.00	0.61
1:A:23:MET:CE	1:A:205:VAL:CG1	2.79	0.61
1:B:325:LYS:O	1:B:329:THR:HG23	2.00	0.61
1:D:213:GLU:O	1:D:217:ASP:HB2	2.01	0.61
1:C:229:LEU:HB3	1:C:409:MET:HE1	1.81	0.61
1:A:223:THR:HG22	1:A:224:ILE:H	1.66	0.61
1:C:404:LYS:CB	1:C:408:GLU:HB2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:CYS:HB2	1:D:160:GLU:OE2	2.01	0.61
1:D:410:ASN:HB3	1:D:418:GLU:OE2	2.01	0.61
1:A:235:LEU:HG	1:A:429:VAL:HG22	1.83	0.61
1:A:223:THR:CG2	1:A:224:ILE:N	2.63	0.60
1:C:3:ASN:N	1:C:6:ASN:HD22	1.98	0.60
1:C:56:MET:HB2	1:C:63:ILE:HD11	1.83	0.60
1:A:450:GLU:HG2	1:C:450:GLU:HG2	1.84	0.60
1:C:154:PRO:CA	1:C:173:THR:HG22	2.30	0.60
1:D:181:ASN:C	1:D:183:PRO:HD3	2.22	0.60
1:D:202:ARG:O	1:D:484:MET:HB3	2.01	0.60
1:A:182:ASP:N	1:A:183:PRO:HD3	2.17	0.60
1:C:110:GLN:O	1:C:114:VAL:HG23	2.02	0.60
1:C:144:ARG:HB2	1:C:147:ILE:HD12	1.84	0.60
1:D:210:PHE:O	1:D:214:VAL:HG23	2.01	0.59
1:B:382:ILE:N	1:B:382:ILE:HD12	1.99	0.59
1:B:408:GLU:O	1:B:412:VAL:HG23	2.02	0.59
1:C:171:VAL:O	1:C:173:THR:HG23	2.02	0.59
1:C:144:ARG:HB2	1:C:147:ILE:CD1	2.32	0.59
1:B:401:ILE:HD11	1:B:409:MET:HE3	1.83	0.59
1:A:276:ARG:NH1	1:C:455:ASN:HD21	2.00	0.59
1:D:70:GLU:O	1:D:74:GLU:HG2	2.02	0.59
1:A:230:GLN:HG3	1:A:406:LEU:HD13	1.85	0.59
1:A:466:ARG:NH2	1:C:466:ARG:HD2	2.17	0.59
1:C:39:LYS:HD3	1:C:62:ASP:OD2	2.02	0.59
1:C:262:THR:CG2	1:C:395:PRO:HA	2.33	0.59
1:D:106:THR:HB	1:D:107:PRO:HD2	1.84	0.59
1:D:113:ASP:O	1:D:117:THR:HG23	2.03	0.59
1:A:400:THR:HG23	1:A:408:GLU:HG3	1.85	0.58
1:A:139:VAL:HG22	1:A:317:MET:HE3	1.86	0.58
1:A:115:VAL:O	1:A:119:GLN:HG3	2.02	0.58
1:D:119:GLN:HA	1:D:122:MET:HE3	1.83	0.58
1:D:170:GLY:O	1:D:203:ALA:HB2	2.03	0.58
1:C:103:ILE:HG22	1:C:105:LEU:HG	1.84	0.58
1:B:400:THR:HG21	1:B:409:MET:HA	1.85	0.58
1:A:57:ARG:HG2	1:A:57:ARG:HH21	1.67	0.58
1:B:25:ARG:HH22	1:B:201:HIS:HD2	1.51	0.58
1:C:119:GLN:HA	1:C:122:MET:HE3	1.86	0.58
1:C:3:ASN:N	3:C:4131:HOH:O	2.35	0.58
1:D:316:MET:SD	1:D:416:THR:HG23	2.44	0.58
1:A:174:LEU:HD23	1:A:174:LEU:C	2.24	0.57
1:D:54:LEU:HD23	1:D:162:ARG:NE	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:TYR:O	1:A:411:VAL:HG23	2.04	0.57
1:B:278:SER:HB3	1:B:450:GLU:HG3	1.86	0.57
1:B:9:ASN:OD1	1:B:12:GLN:HG3	2.03	0.57
1:D:466:ARG:HD3	3:D:4199:HOH:O	2.03	0.57
1:C:91:THR:HG22	1:C:94:GLU:HG2	1.85	0.57
1:D:152:VAL:HG22	1:D:175:ILE:HG22	1.87	0.57
1:A:70:GLU:O	1:A:74:GLU:HG3	2.04	0.57
1:C:230:GLN:HG3	1:C:406:LEU:HD13	1.87	0.57
1:B:215:LYS:HE3	1:B:307:ILE:O	2.04	0.57
1:C:157:PRO:HG3	1:C:397:ILE:HD13	1.87	0.57
1:C:152:VAL:HG22	1:C:175:ILE:HG22	1.87	0.57
1:B:469:ALA:O	1:B:473:VAL:HG23	2.05	0.57
1:A:139:VAL:HG22	1:A:317:MET:HE1	1.86	0.56
1:D:92:TYR:O	1:D:96:ILE:HG12	2.05	0.56
1:D:131:SER:O	1:D:153:ALA:HB2	2.05	0.56
1:B:248:ALA:HA	1:B:343:PRO:O	2.05	0.56
1:C:148:THR:HA	1:C:181:ASN:O	2.05	0.56
1:A:434:PRO:HG2	3:A:4165:HOH:O	2.06	0.56
1:B:400:THR:HG23	1:B:408:GLU:HG3	1.88	0.56
1:D:105:LEU:HD22	1:D:131:SER:HB2	1.88	0.56
1:D:104:ASN:HD21	1:D:111:HIS:CE1	2.23	0.56
1:A:51:ASN:HD21	1:A:159:THR:HG22	1.71	0.56
1:D:57:ARG:HB2	1:D:57:ARG:HH21	1.71	0.56
1:A:178:HIS:HE1	3:A:4271:HOH:O	1.88	0.56
1:C:224:ILE:O	1:C:224:ILE:HD13	2.06	0.56
1:C:440:GLN:HB3	1:C:441:PRO:HD2	1.88	0.56
1:C:283:LEU:HD13	1:C:457:GLN:NE2	2.20	0.56
1:A:246:ASP:OD1	1:A:247:PRO:HD2	2.06	0.56
1:D:408:GLU:O	1:D:412:VAL:HG23	2.06	0.55
1:A:106:THR:O	1:A:111:HIS:CE1	2.58	0.55
1:B:143:ILE:N	1:B:143:ILE:HD12	2.21	0.55
1:B:297:ALA:HB3	1:B:298:PRO:CD	2.36	0.55
1:C:55:ASN:HD21	1:C:165:TYR:HB2	1.71	0.55
1:B:327:LEU:HD13	1:B:328:LEU:HD23	1.88	0.55
1:A:304:MET:HG3	3:A:4160:HOH:O	2.06	0.55
1:D:401:ILE:C	1:D:403:ARG:H	2.09	0.55
1:C:408:GLU:O	1:C:411:VAL:HG12	2.06	0.55
1:D:240:LEU:HD21	1:D:444:LEU:HG	1.89	0.55
1:C:174:LEU:HD23	1:C:174:LEU:O	2.07	0.55
1:D:370:GLU:O	1:D:374:GLU:HG3	2.07	0.55
1:A:272:LEU:HD21	1:C:455:ASN:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ILE:HD12	1:C:143:ILE:N	2.22	0.55
1:A:102:VAL:HG11	1:A:118:VAL:HG11	1.88	0.55
1:C:23:MET:HE3	1:C:205:VAL:CG1	2.37	0.54
1:A:382:ILE:CD1	1:A:382:ILE:H	2.06	0.54
1:D:265:LEU:CD2	1:D:394:LEU:HD23	2.37	0.54
1:D:293:LYS:HG2	1:D:367:ALA:HB1	1.90	0.54
1:C:132:HIS:CD2	1:C:134:PHE:HB2	2.42	0.54
1:D:418:GLU:HG2	1:D:422:TYR:CZ	2.42	0.54
1:B:156:CYS:SG	1:B:161:VAL:HB	2.47	0.54
1:D:221:GLU:HA	1:D:225:LEU:HB2	1.88	0.54
1:C:249:TYR:HA	1:C:345:TYR:HB2	1.90	0.54
1:D:9:ASN:O	1:D:13:GLN:HG3	2.08	0.54
1:C:38:LYS:HB3	1:C:100:ASP:OD2	2.08	0.54
1:A:311:GLU:HG3	3:A:4174:HOH:O	2.08	0.54
1:D:248:ALA:HA	1:D:343:PRO:O	2.08	0.53
1:B:102:VAL:O	1:B:103:ILE:HD13	2.08	0.53
1:D:403:ARG:HD2	1:D:408:GLU:OE2	2.09	0.53
1:C:224:ILE:C	1:C:224:ILE:HD13	2.28	0.53
1:B:151:MET:HE1	1:B:213:GLU:HG3	1.88	0.53
1:C:224:ILE:HA	1:C:228:MET:HB2	1.90	0.53
1:B:96:ILE:N	1:B:97:PRO:HD2	2.24	0.53
1:D:230:GLN:HG3	1:D:406:LEU:HD13	1.90	0.53
1:B:101:LEU:HD21	1:B:103:ILE:HD11	1.90	0.53
1:B:358:GLY:O	1:B:361:MET:HB2	2.09	0.53
1:D:258:TRP:HH2	1:D:364:MET:CE	2.22	0.52
1:B:297:ALA:HA	1:B:371:LEU:HD21	1.91	0.52
1:C:278:SER:CB	1:C:450:GLU:HG3	2.38	0.52
1:D:261:ILE:HB	1:D:273:MET:HE2	1.91	0.52
1:C:114:VAL:O	1:C:118:VAL:HG23	2.08	0.52
1:C:145:LYS:O	1:C:183:PRO:HG3	2.10	0.52
1:D:57:ARG:CB	1:D:57:ARG:HH21	2.22	0.52
1:D:112:SER:O	1:D:116:ARG:HB2	2.08	0.52
1:C:222:GLN:NE2	1:C:303:HIS:ND1	2.55	0.52
1:D:165:TYR:HA	1:D:169:PHE:O	2.10	0.52
1:C:169:PHE:CE1	1:C:485:LYS:HA	2.45	0.52
1:B:104:ASN:ND2	1:B:111:HIS:NE2	2.58	0.52
1:C:418:GLU:HG2	1:C:422:TYR:CE1	2.45	0.52
1:B:168:GLY:O	1:B:202:ARG:HD3	2.10	0.52
1:B:331:ARG:O	1:B:334:THR:HG22	2.09	0.51
1:A:119:GLN:HA	1:A:122:MET:HE3	1.92	0.51
1:C:104:ASN:HD21	1:C:111:HIS:CD2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ARG:HB2	1:C:147:ILE:HG13	1.91	0.51
1:A:93:GLU:HA	1:A:121:LEU:HD13	1.92	0.51
1:D:404:LYS:CB	1:D:408:GLU:HB2	2.39	0.51
1:C:224:ILE:HD11	1:C:394:LEU:HD22	1.92	0.51
1:A:427:ALA:O	1:A:430:PRO:HD2	2.09	0.51
1:D:261:ILE:HG22	1:D:355:PHE:CD2	2.46	0.51
1:C:408:GLU:O	1:C:412:VAL:HG23	2.10	0.51
1:D:400:THR:HG23	1:D:408:GLU:HG3	1.93	0.51
1:D:144:ARG:HB3	1:D:147:ILE:HG13	1.93	0.51
1:B:221:GLU:HA	1:B:225:LEU:HB2	1.93	0.51
1:A:455:ASN:HD21	1:C:276:ARG:NH1	1.97	0.51
1:C:63:ILE:HB	1:C:87:PHE:HE1	1.76	0.51
1:A:57:ARG:NH2	1:A:57:ARG:HG2	2.26	0.51
1:C:27:GLU:O	1:C:192:LYS:HE3	2.12	0.51
1:A:265:LEU:HG	1:A:391:LEU:HD11	1.91	0.51
1:C:80:ARG:O	1:C:84:GLU:HG3	2.11	0.50
1:C:144:ARG:HB2	1:C:147:ILE:CG1	2.41	0.50
1:B:162:ARG:HH21	1:B:166:LYS:CE	2.23	0.50
1:A:483:ASP:O	1:A:486:ARG:HB3	2.11	0.50
1:C:35:LEU:HD23	1:C:193:ALA:HB3	1.94	0.50
1:B:106:THR:HB	1:B:107:PRO:HD2	1.93	0.50
1:B:455:ASN:ND2	1:D:276:ARG:HH11	2.03	0.50
1:D:35:LEU:HD21	1:D:190:ILE:HG23	1.94	0.50
1:C:61:LEU:O	1:C:63:ILE:HG13	2.11	0.50
1:B:461:VAL:O	1:B:465:ILE:HG13	2.11	0.50
1:B:486:ARG:NH2	1:B:486:ARG:HB2	2.27	0.50
1:B:16:GLN:HB3	1:B:211:VAL:HB	1.93	0.50
1:C:109:LYS:HA	1:C:320:TRP:CZ3	2.47	0.50
1:B:119:GLN:HA	1:B:122:MET:HE3	1.93	0.50
1:B:109:LYS:HA	1:B:320:TRP:CH2	2.47	0.50
1:C:183:PRO:C	1:C:185:GLY:H	2.14	0.49
1:A:258:TRP:HH2	1:A:364:MET:HE3	1.77	0.49
1:D:53:GLY:HA3	1:D:65:TYR:OH	2.11	0.49
1:A:376:MET:CE	1:A:390:SER:HB3	2.42	0.49
1:C:262:THR:HG23	1:C:395:PRO:HA	1.94	0.49
1:D:118:VAL:O	1:D:122:MET:HG3	2.12	0.49
1:C:23:MET:HE2	1:C:205:VAL:O	2.12	0.49
1:D:333:GLU:O	1:D:337:THR:HG23	2.12	0.49
1:C:382:ILE:H	1:C:382:ILE:CD1	1.94	0.49
1:C:277:LEU:HD11	1:C:362:ILE:HD12	1.93	0.49
1:A:148:THR:HA	1:A:181:ASN:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:GLU:N	3:C:4223:HOH:O	2.45	0.49
1:A:116:ARG:HH11	1:A:116:ARG:HG3	1.77	0.49
1:B:246:ASP:OD2	1:B:248:ALA:HB3	2.13	0.49
1:A:210:PHE:O	1:A:214:VAL:HG23	2.13	0.49
1:A:53:GLY:HA3	1:A:65:TYR:OH	2.12	0.49
1:C:96:ILE:N	1:C:97:PRO:HD2	2.27	0.49
1:C:248:ALA:HA	1:C:343:PRO:O	2.12	0.49
1:A:184:LYS:HB2	1:A:186:GLU:HG2	1.94	0.49
1:B:486:ARG:CB	1:B:486:ARG:HH21	2.25	0.49
1:C:427:ALA:O	1:C:430:PRO:HD2	2.12	0.49
1:B:279:ASN:N	1:B:280:PRO:HD2	2.28	0.49
1:D:93:GLU:H	1:D:93:GLU:CD	2.14	0.49
1:C:298:PRO:HG2	3:C:4145:HOH:O	2.13	0.49
1:C:123:LYS:O	1:C:144:ARG:NH2	2.46	0.49
1:B:292:LEU:HD21	1:B:364:MET:HG2	1.94	0.49
1:D:182:ASP:N	1:D:183:PRO:HD3	2.28	0.49
1:D:174:LEU:HD23	1:D:174:LEU:C	2.33	0.49
1:C:289:SER:O	1:C:293:LYS:HG3	2.13	0.49
1:C:68:ARG:O	1:C:72:ILE:HG13	2.13	0.49
1:B:273:MET:CE	1:B:365:VAL:HG11	2.43	0.48
1:B:382:ILE:N	1:B:382:ILE:CD1	2.68	0.48
1:C:265:LEU:HD13	1:C:273:MET:HE3	1.95	0.48
1:B:162:ARG:HH21	1:B:166:LYS:HE2	1.78	0.48
1:C:224:ILE:HG23	1:C:225:LEU:N	2.28	0.48
1:A:276:ARG:HD3	1:C:455:ASN:ND2	2.29	0.48
1:B:278:SER:CB	1:B:450:GLU:HG3	2.43	0.48
1:A:57:ARG:CB	1:A:57:ARG:HH21	2.26	0.48
1:B:23:MET:HE3	1:B:205:VAL:HB	1.94	0.48
1:C:102:VAL:O	1:C:128:LEU:HD12	2.14	0.48
1:A:51:ASN:ND2	1:A:159:THR:HG22	2.28	0.48
1:D:63:ILE:N	1:D:63:ILE:HD12	2.29	0.48
1:B:174:LEU:C	1:B:174:LEU:HD23	2.34	0.48
1:D:387:TYR:CD2	1:D:477:LEU:HD12	2.48	0.48
1:B:265:LEU:HD13	1:B:273:MET:HE3	1.95	0.48
1:A:115:VAL:HG12	1:A:119:GLN:HE21	1.78	0.48
1:B:224:ILE:HD13	1:B:224:ILE:O	2.13	0.48
1:D:327:LEU:HD22	1:D:327:LEU:O	2.13	0.48
1:C:483:ASP:O	1:C:487:ILE:HG13	2.14	0.48
1:D:359:VAL:HB	1:D:443:ASP:O	2.14	0.48
1:C:376:MET:CE	1:C:390:SER:HB3	2.43	0.48
1:C:182:ASP:N	1:C:183:PRO:HD3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:LEU:O	1:C:391:LEU:HD12	2.14	0.48
1:D:265:LEU:HG	1:D:391:LEU:CD1	2.44	0.47
1:A:468:HIS:ND1	1:A:470:ILE:HG22	2.28	0.47
1:C:56:MET:HB2	1:C:63:ILE:CD1	2.43	0.47
1:B:427:ALA:C	1:B:430:PRO:HD2	2.34	0.47
1:D:119:GLN:HA	1:D:122:MET:CE	2.44	0.47
1:D:161:VAL:HG13	1:D:162:ARG:N	2.28	0.47
1:A:440:GLN:HB3	1:A:441:PRO:HD2	1.96	0.47
1:C:262:THR:HG21	1:C:398:ALA:CB	2.44	0.47
1:D:244:GLY:O	1:D:245:THR:O	2.32	0.47
1:B:3:ASN:HB3	1:B:6:ASN:HD22	1.79	0.47
1:A:132:HIS:CD2	1:A:134:PHE:HB2	2.49	0.47
1:D:51:ASN:HD22	1:D:52:GLN:HG3	1.80	0.47
1:D:156:CYS:HB2	1:D:160:GLU:CD	2.34	0.47
1:B:483:ASP:OD1	1:B:486:ARG:NH2	2.47	0.47
1:D:28:PHE:CD2	1:D:201:HIS:HB3	2.50	0.47
1:C:98:GLN:HA	1:C:123:LYS:HD3	1.95	0.47
1:B:265:LEU:HG	1:B:391:LEU:HD11	1.96	0.47
1:B:119:GLN:HA	1:B:122:MET:CE	2.45	0.47
1:C:10:LEU:O	1:C:14:LEU:HD13	2.14	0.47
1:C:365:VAL:HG13	1:C:394:LEU:HD21	1.97	0.47
1:C:35:LEU:HD23	1:C:193:ALA:CB	2.43	0.47
1:C:51:ASN:HD21	1:C:159:THR:HB	1.78	0.47
1:A:16:GLN:HB3	1:A:211:VAL:HB	1.97	0.47
1:C:106:THR:HB	1:C:107:PRO:HD2	1.97	0.47
1:D:249:TYR:HA	1:D:345:TYR:HB2	1.97	0.47
1:C:287:ALA:O	1:C:291:GLN:HG3	2.14	0.47
1:D:3:ASN:O	1:D:7:THR:HG23	2.15	0.47
1:C:9:ASN:O	1:C:10:LEU:C	2.54	0.47
1:A:174:LEU:HD23	1:A:175:ILE:N	2.30	0.47
1:C:218:LEU:O	1:C:222:GLN:HG2	2.15	0.47
1:A:287:ALA:O	1:A:291:GLN:HG3	2.15	0.47
1:A:384:GLU:HG3	1:A:477:LEU:HD11	1.97	0.47
1:C:119:GLN:HA	1:C:122:MET:CE	2.45	0.46
1:C:97:PRO:O	1:C:98:GLN:HB2	2.15	0.46
1:B:391:LEU:O	1:B:391:LEU:HD12	2.15	0.46
1:B:230:GLN:HG3	1:B:406:LEU:CD1	2.44	0.46
1:B:261:ILE:HD13	1:B:362:ILE:HG12	1.97	0.46
1:B:223:THR:CG2	1:B:300:PHE:CE2	2.98	0.46
1:D:10:LEU:HD23	1:D:14:LEU:HD22	1.97	0.46
1:D:115:VAL:O	1:D:119:GLN:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:PHE:CG	1:A:170:GLY:N	2.82	0.46
1:C:327:LEU:HD22	1:C:327:LEU:O	2.15	0.46
1:B:148:THR:HG23	1:B:182:ASP:HA	1.97	0.46
1:C:317:MET:O	1:C:320:TRP:HB2	2.14	0.46
1:C:468:HIS:O	1:C:472:GLN:HG2	2.15	0.46
1:D:95:LEU:C	1:D:97:PRO:HD2	2.35	0.46
1:A:49:GLY:HA2	1:A:105:LEU:HD12	1.97	0.46
1:C:68:ARG:HG3	1:C:70:GLU:OE1	2.16	0.46
1:D:196:ALA:HA	1:D:201:HIS:ND1	2.31	0.46
1:D:219:MET:HG2	1:D:304:MET:SD	2.56	0.46
1:D:255:GLN:NE2	1:D:256:PHE:CE2	2.84	0.46
1:C:91:THR:CG2	1:C:94:GLU:HG2	2.46	0.46
1:B:244:GLY:O	1:B:245:THR:C	2.54	0.46
1:A:225:LEU:O	1:A:397:ILE:HG21	2.15	0.46
1:C:217:ASP:HA	1:C:389:GLU:OE1	2.15	0.46
1:B:304:MET:O	1:B:308:ILE:HG12	2.15	0.46
1:D:60:GLY:O	1:D:61:LEU:HD23	2.16	0.46
1:C:332:GLU:O	1:C:336:LYS:HG2	2.16	0.46
1:A:450:GLU:HG2	1:C:450:GLU:CG	2.45	0.46
1:A:248:ALA:HA	1:A:343:PRO:O	2.16	0.46
1:C:71:ALA:HA	1:C:76:ARG:HD2	1.97	0.46
1:B:138:GLU:OE2	1:B:313:SER:HB3	2.16	0.46
1:A:96:ILE:N	1:A:97:PRO:CD	2.77	0.46
1:A:181:ASN:C	1:A:183:PRO:HD3	2.36	0.46
1:D:334:THR:O	1:D:340:GLU:HG3	2.16	0.46
1:C:265:LEU:HB2	1:C:273:MET:HE2	1.98	0.45
1:B:427:ALA:O	1:B:430:PRO:HD2	2.16	0.45
1:B:175:ILE:O	1:B:175:ILE:HG13	2.15	0.45
1:A:88:LYS:HZ2	1:A:95:LEU:HD21	1.81	0.45
1:D:143:ILE:HG22	1:D:181:ASN:ND2	2.31	0.45
1:B:313:SER:O	1:B:317:MET:HG3	2.16	0.45
1:B:394:LEU:HB3	1:B:395:PRO:HD3	1.98	0.45
1:B:122:MET:O	1:B:144:ARG:NH2	2.50	0.45
1:C:221:GLU:HA	1:C:225:LEU:HB2	1.98	0.45
1:A:126:ALA:O	1:A:147:ILE:HG23	2.17	0.45
1:B:401:ILE:HD11	1:B:409:MET:HE2	1.99	0.45
1:C:181:ASN:C	1:C:183:PRO:HD3	2.36	0.45
1:D:13:GLN:O	1:D:17:LEU:HB2	2.15	0.45
1:B:139:VAL:O	1:B:141:GLU:N	2.42	0.45
1:B:463:GLU:O	1:B:467:SER:HB3	2.16	0.45
1:D:346:GLU:HA	1:D:346:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:PRO:HA	1:A:121:LEU:O	2.17	0.45
1:B:173:THR:O	1:B:205:VAL:HA	2.15	0.45
1:A:487:ILE:HG22	1:A:487:ILE:O	2.16	0.45
1:C:115:VAL:C	1:C:117:THR:H	2.20	0.45
1:C:258:TRP:HB2	3:C:4223:HOH:O	2.16	0.45
1:D:111:HIS:HB2	3:D:4145:HOH:O	2.17	0.45
1:A:229:LEU:HA	1:A:229:LEU:HD12	1.81	0.45
1:B:139:VAL:HG22	1:B:317:MET:CE	2.45	0.45
1:D:480:TYR:O	1:D:482:THR:N	2.49	0.45
1:B:345:TYR:CE1	1:B:347:GLY:HA3	2.52	0.45
1:B:218:LEU:O	1:B:222:GLN:HG2	2.16	0.45
1:D:58:ASP:HB2	1:D:165:TYR:HE2	1.82	0.45
1:D:63:ILE:H	1:D:63:ILE:HD12	1.82	0.45
1:A:463:GLU:O	1:A:467:SER:CB	2.64	0.45
1:B:281:ALA:HA	1:B:448:ILE:HD12	1.99	0.45
1:D:173:THR:O	1:D:205:VAL:HA	2.17	0.45
1:D:251:GLU:HG2	1:D:343:PRO:O	2.17	0.45
1:D:291:GLN:HE21	1:D:435:PHE:HE1	1.65	0.45
1:A:325:LYS:HE3	1:A:329:THR:HG21	1.98	0.45
1:D:450:GLU:H	1:D:450:GLU:CD	2.20	0.45
1:D:160:GLU:CD	1:D:160:GLU:H	2.21	0.45
1:A:177:VAL:HG21	1:A:187:GLY:HA3	1.99	0.45
1:C:262:THR:HG21	1:C:395:PRO:HA	1.99	0.45
1:D:397:ILE:O	1:D:400:THR:HB	2.17	0.45
1:D:151:MET:O	1:D:175:ILE:HA	2.17	0.45
1:C:159:THR:O	1:C:163:GLU:HG3	2.17	0.45
1:C:196:ALA:HA	1:C:201:HIS:ND1	2.32	0.45
1:C:66:ALA:HB1	1:C:92:TYR:HD2	1.81	0.45
1:B:400:THR:CG2	1:B:409:MET:HA	2.47	0.44
1:C:259:GLU:O	1:C:262:THR:HG22	2.17	0.44
1:A:10:LEU:HD13	1:A:14:LEU:HD22	1.99	0.44
1:A:119:GLN:HA	1:A:122:MET:CE	2.47	0.44
1:A:391:LEU:HD12	1:A:391:LEU:O	2.17	0.44
1:B:265:LEU:HD21	1:B:391:LEU:CD1	2.47	0.44
1:B:104:ASN:ND2	1:B:111:HIS:CD2	2.86	0.44
1:B:413:ILE:HB	1:B:417:ALA:CB	2.48	0.44
1:A:83:THR:HG22	1:A:89:VAL:HG11	1.99	0.44
1:C:118:VAL:O	1:C:122:MET:HG3	2.17	0.44
1:B:288:LEU:O	1:B:292:LEU:HB2	2.18	0.44
1:D:96:ILE:N	1:D:97:PRO:CD	2.77	0.44
1:C:327:LEU:HD11	1:C:331:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:SER:O	1:A:36:GLN:HB2	2.18	0.44
1:C:49:GLY:HA2	1:C:105:LEU:CD1	2.48	0.44
1:B:316:MET:HB2	1:B:419:TYR:CE2	2.53	0.44
1:A:23:MET:HE3	1:A:205:VAL:HB	2.00	0.44
1:D:145:LYS:O	1:D:183:PRO:HG3	2.18	0.44
1:D:391:LEU:O	1:D:391:LEU:HD12	2.17	0.44
1:D:17:LEU:CD1	1:D:211:VAL:HG12	2.48	0.44
1:C:218:LEU:HD13	1:C:312:PHE:CE2	2.52	0.44
1:C:71:ALA:HA	1:C:76:ARG:CD	2.48	0.44
1:A:316:MET:CE	1:A:416:THR:HG23	2.48	0.44
1:B:255:GLN:HG3	1:B:402:ALA:HA	2.00	0.44
1:B:330:TRP:CD1	1:B:426:TYR:CE2	3.06	0.44
1:C:143:ILE:CD1	1:C:143:ILE:N	2.80	0.44
1:A:359:VAL:HG23	3:A:4137:HOH:O	2.17	0.44
1:C:292:LEU:HD13	1:C:435:PHE:CZ	2.53	0.44
1:A:52:GLN:O	1:A:56:MET:HG3	2.18	0.44
1:D:316:MET:CE	1:D:416:THR:HG23	2.48	0.43
1:D:249:TYR:OH	1:D:353:GLU:OE1	2.35	0.43
1:C:229:LEU:HA	1:C:229:LEU:HD12	1.84	0.43
1:C:96:ILE:CG2	1:C:121:LEU:HB2	2.48	0.43
1:C:54:LEU:HB3	1:C:162:ARG:HH11	1.82	0.43
1:B:188:MET:O	1:B:192:LYS:HG3	2.17	0.43
1:A:455:ASN:ND2	1:C:276:ARG:NH1	2.63	0.43
1:A:400:THR:CG2	1:A:409:MET:HA	2.45	0.43
1:A:57:ARG:HH21	1:A:57:ARG:HB3	1.84	0.43
1:D:410:ASN:HB3	1:D:418:GLU:HG3	2.00	0.43
1:C:427:ALA:C	1:C:430:PRO:HD2	2.39	0.43
1:B:446:LYS:HG2	1:B:447:ALA:H	1.82	0.43
1:A:156:CYS:HB2	1:A:160:GLU:CG	2.48	0.43
1:B:157:PRO:HG2	1:B:158:GLY:H	1.83	0.43
1:B:118:VAL:O	1:B:122:MET:HG3	2.17	0.43
1:B:303:HIS:O	1:B:307:ILE:HG13	2.18	0.43
1:B:327:LEU:HD22	1:B:327:LEU:O	2.18	0.43
1:A:52:GLN:HB3	1:A:56:MET:HE2	2.00	0.43
1:B:177:VAL:HG21	1:B:187:GLY:HA3	2.00	0.43
1:D:89:VAL:HG12	1:D:89:VAL:O	2.18	0.43
1:C:392:HIS:O	1:C:395:PRO:HD2	2.19	0.43
1:C:142:GLN:C	1:C:143:ILE:HD12	2.39	0.43
1:C:67:LEU:HD22	1:C:78:SER:HB2	2.00	0.43
1:A:325:LYS:O	1:A:329:THR:HG23	2.19	0.43
1:D:286:TYR:O	1:D:289:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:GLU:HG2	1:C:450:GLU:CD	2.39	0.43
1:D:427:ALA:O	1:D:430:PRO:HD2	2.19	0.43
1:C:50:LEU:HG	1:C:54:LEU:HD11	2.00	0.43
1:B:215:LYS:HE3	1:B:308:ILE:HA	2.01	0.43
1:D:215:LYS:HG2	1:D:308:ILE:HD13	2.01	0.43
1:B:179:PRO:HB2	1:B:180:GLU:OE1	2.18	0.43
1:B:225:LEU:HB3	1:B:397:ILE:HD12	2.00	0.43
1:D:35:LEU:HG	1:D:193:ALA:CB	2.49	0.43
1:D:407:TYR:O	1:D:411:VAL:HG23	2.18	0.43
1:A:346:GLU:HA	1:A:346:GLU:OE1	2.19	0.43
1:C:397:ILE:CG2	1:C:409:MET:HE2	2.49	0.42
1:C:9:ASN:OD1	1:C:12:GLN:CG	2.65	0.42
1:C:91:THR:H	1:C:94:GLU:HG2	1.84	0.42
1:D:293:LYS:HD3	1:D:367:ALA:HA	2.00	0.42
1:D:219:MET:CG	1:D:304:MET:SD	3.07	0.42
1:C:377:VAL:C	1:C:379:SER:H	2.23	0.42
1:B:459:ARG:HB2	1:D:272:LEU:HD13	2.00	0.42
1:D:376:MET:CE	1:D:390:SER:HB3	2.49	0.42
1:A:433:LYS:HB3	1:A:434:PRO:CD	2.49	0.42
1:A:61:LEU:HB3	1:A:63:ILE:CD1	2.49	0.42
1:A:171:VAL:HG12	1:A:172:PRO:O	2.19	0.42
1:D:224:ILE:HD13	1:D:394:LEU:HD13	2.01	0.42
1:A:345:TYR:OH	1:A:347:GLY:HA3	2.20	0.42
1:D:332:GLU:HA	1:D:332:GLU:OE1	2.19	0.42
1:C:141:GLU:HG3	1:C:143:ILE:HD11	2.02	0.42
1:C:160:GLU:CD	1:C:160:GLU:H	2.22	0.42
1:B:143:ILE:HG22	1:B:144:ARG:N	2.33	0.42
1:C:215:LYS:HE3	1:C:308:ILE:HA	2.02	0.42
1:C:224:ILE:CD1	1:C:394:LEU:HD22	2.50	0.42
1:D:367:ALA:O	1:D:371:LEU:HB2	2.19	0.42
1:B:433:LYS:N	1:B:434:PRO:HD2	2.34	0.42
1:D:57:ARG:C	1:D:59:SER:H	2.22	0.42
1:C:345:TYR:HE1	1:C:347:GLY:HA3	1.83	0.42
1:B:213:GLU:O	1:B:217:ASP:HB2	2.20	0.42
1:D:58:ASP:HB2	1:D:165:TYR:CE2	2.54	0.42
1:D:394:LEU:HB3	1:D:395:PRO:HD3	2.01	0.42
1:C:49:GLY:HA2	1:C:105:LEU:HD13	2.01	0.42
1:B:483:ASP:O	1:B:487:ILE:HG13	2.19	0.42
1:B:373:PHE:HB2	1:B:470:ILE:HD12	2.01	0.42
1:A:466:ARG:HD2	1:C:466:ARG:NH2	2.34	0.42
1:D:32:ALA:HB1	1:D:61:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LYS:O	1:C:20:CYS:HB2	2.19	0.42
1:C:397:ILE:HG21	1:C:409:MET:HE2	2.02	0.42
1:B:144:ARG:HB2	1:B:147:ILE:HG13	2.00	0.42
1:D:52:GLN:C	1:D:56:MET:HE2	2.40	0.42
1:A:229:LEU:HD23	1:A:397:ILE:HG22	2.02	0.42
1:B:425:SER:O	1:B:429:VAL:HG23	2.20	0.42
1:B:286:TYR:CD1	1:B:461:VAL:HG13	2.55	0.42
1:B:143:ILE:HB	1:B:181:ASN:HD21	1.85	0.42
1:B:253:LEU:O	1:B:257:GLY:N	2.51	0.42
1:B:229:LEU:HA	1:B:229:LEU:HD12	1.78	0.42
1:C:180:GLU:H	1:C:180:GLU:HG2	1.66	0.42
1:B:172:PRO:HA	1:B:204:GLY:O	2.20	0.42
1:B:400:THR:CG2	1:B:408:GLU:HG3	2.50	0.41
1:D:329:THR:O	1:D:332:GLU:HB2	2.20	0.41
1:D:23:MET:SD	1:D:175:ILE:HD11	2.60	0.41
1:A:463:GLU:O	1:A:467:SER:HB2	2.20	0.41
1:B:359:VAL:HG23	3:B:4137:HOH:O	2.19	0.41
1:C:251:GLU:HG3	1:C:344:GLN:HA	2.02	0.41
1:A:18:GLY:O	1:A:382:ILE:HG12	2.20	0.41
1:A:118:VAL:O	1:A:122:MET:HG3	2.20	0.41
1:B:151:MET:HE1	1:B:213:GLU:CG	2.50	0.41
1:B:396:LEU:HA	1:B:399:ASN:ND2	2.35	0.41
1:D:154:PRO:CB	1:D:173:THR:HG22	2.51	0.41
1:C:96:ILE:HG21	1:C:121:LEU:HB2	2.01	0.41
1:B:330:TRP:HB3	1:B:422:TYR:CG	2.56	0.41
1:B:14:LEU:HD11	1:C:14:LEU:HD11	2.02	0.41
1:D:57:ARG:NH2	1:D:87:PHE:CE2	2.88	0.41
1:B:103:ILE:HG22	1:B:105:LEU:HG	2.01	0.41
1:C:273:MET:SD	1:C:362:ILE:HG23	2.60	0.41
1:D:463:GLU:O	1:D:467:SER:CB	2.69	0.41
1:A:56:MET:O	1:A:61:LEU:HB2	2.20	0.41
1:D:328:LEU:O	1:D:331:ARG:HB2	2.20	0.41
1:A:116:ARG:HG3	1:A:116:ARG:NH1	2.35	0.41
1:D:429:VAL:CB	1:D:430:PRO:HD3	2.48	0.41
1:C:50:LEU:O	1:C:54:LEU:HG	2.21	0.41
1:D:109:LYS:HG2	1:D:109:LYS:O	2.20	0.41
1:D:258:TRP:O	1:D:262:THR:HG23	2.21	0.41
1:B:144:ARG:HB3	1:B:146:ASP:OD1	2.20	0.41
1:D:235:LEU:HD11	1:D:429:VAL:HA	2.02	0.41
1:C:50:LEU:HG	1:C:54:LEU:CD1	2.50	0.41
1:C:248:ALA:O	1:C:345:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ASN:HD21	1:B:111:HIS:CD2	2.38	0.41
1:D:480:TYR:C	1:D:482:THR:N	2.74	0.41
1:B:440:GLN:HB3	1:B:441:PRO:HD2	2.03	0.41
1:B:273:MET:HE3	1:B:365:VAL:HG11	2.03	0.41
1:A:14:LEU:HD12	1:A:14:LEU:HA	1.96	0.41
1:B:253:LEU:HA	1:B:253:LEU:HD23	1.87	0.41
1:B:384:GLU:HB3	1:B:477:LEU:HD11	2.03	0.41
1:A:81:LYS:O	1:A:85:ASN:ND2	2.51	0.41
1:C:262:THR:O	1:C:265:LEU:HB3	2.21	0.40
1:C:221:GLU:OE2	1:C:417:ALA:HA	2.21	0.40
1:D:186:GLU:O	1:D:190:ILE:HG13	2.21	0.40
1:A:376:MET:HE1	1:A:390:SER:HB3	2.01	0.40
1:B:173:THR:O	1:B:205:VAL:HG13	2.21	0.40
1:B:173:THR:HG23	1:B:205:VAL:HG13	2.04	0.40
1:A:83:THR:CG2	1:A:89:VAL:HG11	2.50	0.40
1:D:19:LYS:O	1:D:208:SER:HA	2.21	0.40
1:B:369:VAL:HG13	1:B:390:SER:O	2.21	0.40
1:A:109:LYS:HG3	1:A:320:TRP:CG	2.57	0.40
1:C:384:GLU:H	1:C:384:GLU:HG2	1.58	0.40
1:D:102:VAL:HG11	1:D:118:VAL:HG11	2.04	0.40
1:B:392:HIS:O	1:B:395:PRO:HD2	2.21	0.40
1:C:139:VAL:O	1:C:141:GLU:N	2.48	0.40
1:B:413:ILE:HB	1:B:417:ALA:HB3	2.03	0.40
1:C:268:GLY:HA3	1:C:272:LEU:HB2	2.03	0.40
1:A:345:TYR:CZ	1:A:347:GLY:CA	3.01	0.40
1:B:358:GLY:O	1:B:361:MET:N	2.53	0.40
1:A:446:LYS:HG2	1:A:447:ALA:N	2.35	0.40
1:D:250:ALA:O	1:D:253:LEU:N	2.55	0.40
1:C:297:ALA:HA	1:C:371:LEU:HD21	2.03	0.40
1:C:112:SER:O	1:C:116:ARG:HG3	2.21	0.40
1:B:222:GLN:NE2	1:B:303:HIS:ND1	2.63	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	485/491 (99%)	457 (94%)	27 (6%)	1 (0%)	52 77
1	B	427/491 (87%)	379 (89%)	38 (9%)	10 (2%)	8 14
1	C	485/491 (99%)	425 (88%)	54 (11%)	6 (1%)	16 33
1	D	464/491 (94%)	409 (88%)	46 (10%)	9 (2%)	10 19
All	All	1861/1964 (95%)	1670 (90%)	165 (9%)	26 (1%)	14 28

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	20	CYS
1	D	245	THR
1	B	245	THR
1	D	92	TYR
1	D	145	LYS
1	C	183	PRO
1	B	169	PHE
1	B	180	GLU
1	B	439	LEU
1	C	184	LYS
1	D	481	MET
1	A	391	LEU
1	B	179	PRO
1	B	325	LYS
1	B	391	LEU
1	C	10	LEU
1	D	332	GLU
1	D	402	ALA
1	B	324	ASP
1	C	75	LYS
1	D	183	PRO
1	B	158	GLY
1	C	44	GLY
1	D	89	VAL
1	D	72	ILE
1	B	157	PRO

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	393/395 (100%)	375 (95%)	18 (5%)	33	61
1	B	345/395 (87%)	335 (97%)	10 (3%)	50	77
1	C	390/395 (99%)	374 (96%)	16 (4%)	37	66
1	D	375/395 (95%)	356 (95%)	19 (5%)	29	55
All	All	1503/1580 (95%)	1440 (96%)	63 (4%)	36	65

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	17	LEU
1	A	36	GLN
1	A	57	ARG
1	A	61	LEU
1	A	111	HIS
1	A	131	SER
1	A	180	GLU
1	A	223	THR
1	A	224	ILE
1	A	229	LEU
1	A	251	GLU
1	A	253	LEU
1	A	292	LEU
1	A	322	ASN
1	A	382	ILE
1	A	425	SER
1	A	432	LEU
1	B	17	LEU
1	B	26	ASP
1	B	110	GLN
1	B	174	LEU
1	B	180	GLU
1	B	224	ILE

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Mol	Chain	Res	Type
1	B	229	LEU
1	B	251	GLU
1	B	322	ASN
1	B	382	ILE
1	C	10	LEU
1	C	57	ARG
1	C	68	ARG
1	C	87	PHE
1	C	111	HIS
1	C	224	ILE
1	C	229	LEU
1	C	251	GLU
1	C	262	THR
1	C	292	LEU
1	C	301	GLN
1	C	322	ASN
1	C	327	LEU
1	C	382	ILE
1	C	384	GLU
1	C	486	ARG
1	D	14	LEU
1	D	17	LEU
1	D	51	ASN
1	D	57	ARG
1	D	93	GLU
1	D	104	ASN
1	D	110	GLN
1	D	112	SER
1	D	219	MET
1	D	223	THR
1	D	224	ILE
1	D	251	GLU
1	D	322	ASN
1	D	331	ARG
1	D	382	ILE
1	D	384	GLU
1	D	415	ASP
1	D	432	LEU
1	D	466	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	48	GLN
1	A	51	ASN
1	A	110	GLN
1	A	111	HIS
1	A	178	HIS
1	A	322	ASN
1	A	344	GLN
1	A	455	ASN
1	A	457	GLN
1	B	6	ASN
1	B	36	GLN
1	B	104	ASN
1	B	110	GLN
1	B	132	HIS
1	B	142	GLN
1	B	222	GLN
1	B	301	GLN
1	B	322	ASN
1	B	344	GLN
1	B	455	ASN
1	B	457	GLN
1	B	462	ASN
1	C	36	GLN
1	C	51	ASN
1	C	110	GLN
1	C	111	HIS
1	C	135	ASN
1	C	222	GLN
1	C	322	ASN
1	C	455	ASN
1	C	457	GLN
1	C	462	ASN
1	D	110	GLN
1	D	178	HIS
1	D	181	ASN
1	D	291	GLN
1	D	322	ASN
1	D	344	GLN
1	D	399	ASN
1	D	455	ASN
1	D	457	GLN
1	D	462	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

9 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	A	4121	-	4,4,4	0.22	0	6,6,6	0.15	0
2	SO4	A	4122	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	A	4127	-	4,4,4	0.23	0	6,6,6	0.16	0
2	SO4	A	4128	-	4,4,4	0.25	0	6,6,6	0.11	0
2	SO4	B	4126	-	4,4,4	0.24	0	6,6,6	5.24	6 (100%)
2	SO4	C	4125	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	D	4123	-	4,4,4	0.25	0	6,6,6	0.17	0
2	SO4	D	4124	-	4,4,4	0.27	0	6,6,6	0.07	0
2	SO4	D	4129	-	4,4,4	0.26	0	6,6,6	0.08	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	SO4	A	4121	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	4122	-	-	0/0/0/0	0/0/0/0
2	SO4	A	4127	-	-	0/0/0/0	0/0/0/0
2	SO4	A	4128	-	-	0/0/0/0	0/0/0/0
2	SO4	B	4126	-	-	0/0/0/0	0/0/0/0
2	SO4	C	4125	-	-	0/0/0/0	0/0/0/0
2	SO4	D	4123	-	-	0/0/0/0	0/0/0/0
2	SO4	D	4124	-	-	0/0/0/0	0/0/0/0
2	SO4	D	4129	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	4126	SO4	O2-S-O1	-9.27	80.11	109.50
2	B	4126	SO4	O4-S-O3	-6.88	80.99	108.98
2	B	4126	SO4	O3-S-O2	-3.29	79.58	110.19
2	B	4126	SO4	O4-S-O1	-3.18	80.58	110.19
2	B	4126	SO4	O4-S-O2	2.22	130.85	110.19
2	B	4126	SO4	O3-S-O1	2.37	132.27	110.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	487/491 (99%)	-0.57	1 (0%)	95	95	17, 32, 55, 76	0
1	B	431/491 (87%)	-0.06	14 (3%)	51	44	26, 54, 91, 115	0
1	C	487/491 (99%)	-0.19	13 (2%)	58	51	22, 47, 88, 95	0
1	D	470/491 (95%)	-0.17	13 (2%)	56	49	23, 49, 82, 104	0
All	All	1875/1964 (95%)	-0.25	41 (2%)	65	59	17, 44, 87, 115	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	486	ARG	4.1
1	B	121	LEU	4.1
1	D	73	ALA	4.0
1	B	98	GLN	3.8
1	C	79	TRP	3.6
1	D	486	ARG	3.4
1	C	73	ALA	3.3
1	C	131	SER	3.1
1	D	159	THR	2.9
1	C	72	ILE	2.8
1	B	110	GLN	2.7
1	C	87	PHE	2.7
1	B	167	ARG	2.7
1	D	407	TYR	2.6
1	B	126	ALA	2.6
1	B	122	MET	2.6
1	D	87	PHE	2.5
1	C	489	VAL	2.5
1	B	95	LEU	2.5
1	C	167	ARG	2.5
1	B	224	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	29	ALA	2.4
1	B	120	PRO	2.4
1	D	224	ILE	2.4
1	B	147	ILE	2.3
1	B	321	ALA	2.3
1	D	72	ILE	2.3
1	D	167	ARG	2.3
1	C	169	PHE	2.2
1	C	152	VAL	2.2
1	D	489	VAL	2.2
1	B	217	ASP	2.2
1	B	132	HIS	2.2
1	B	119	GLN	2.1
1	C	321	ALA	2.1
1	D	74	GLU	2.1
1	C	29	ALA	2.1
1	C	153	ALA	2.1
1	A	220	GLY	2.1
1	D	50	LEU	2.1
1	D	328	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	4127	5/5	0.98	0.12	-0.26	78,78,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	4128	5/5	0.95	0.18	-	93,93,94,94	0
2	SO4	D	4129	5/5	0.84	0.23	-	112,112,113,114	0
2	SO4	D	4123	5/5	0.97	0.10	-	60,61,62,63	0
2	SO4	D	4124	5/5	0.99	0.06	-	49,49,50,51	0
2	SO4	C	4125	5/5	0.97	0.16	-	68,69,69,70	0
2	SO4	A	4122	5/5	0.97	0.07	-	63,64,64,65	0
2	SO4	B	4126	5/5	0.98	0.09	-	86,86,86,86	0
2	SO4	A	4121	5/5	0.98	0.09	-	47,49,50,50	0

6.5 Other polymers

There are no such residues in this entry.