Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 06:11 pm GMT

PDB ID	:	4AQ6
Title	:	substrate bound homogentisate 1,2-dioxygenase
Authors	:	Jeoung, J.-H.; Lin, T.-Y.; Bommer, M.; Dobbek, H.
Deposited on	:	2012-04-12
Resolution	:	1.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

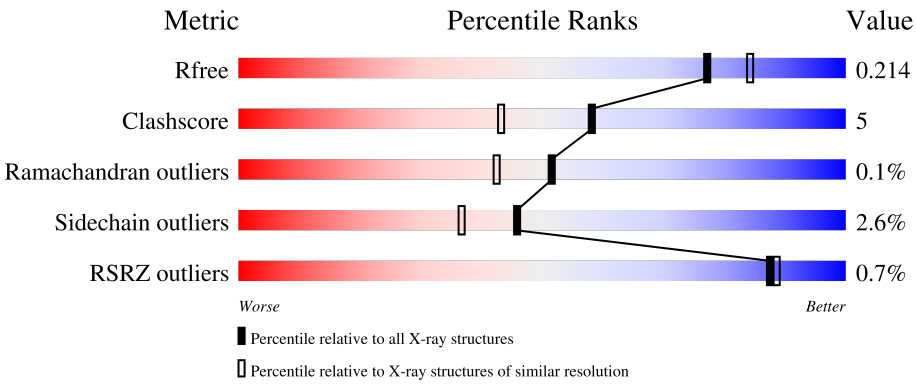
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	433	89% 9% •
1	B	433	% 88% 10% •
1	C	433	87% 10% ••
1	D	433	87% 10% ••
1	E	433	87% 11% ••

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Mol	Chain	Length	Quality of chain
1	F	433	88% 10% •
1	G	433	.% 83% 14% • •
1	H	433	.% 86% 11% • •
1	I	433	2% 83% 15% •
1	J	433	.% 87% 11% •
1	K	433	.% 87% 11% •
1	L	433	.% 88% 9% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 44389 atoms, of which 28 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 HOMOGENTISATE 1,2-DIOXYGENASE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	425	Total C H N O S 3311 2115 2 580 597 17	0	1	0
1	B	425	Total C N O S 3300 2110 580 593 17	0	1	0
1	C	425	Total C N O S 3298 2109 576 596 17	0	0	0
1	D	427	Total C N O S 3313 2117 579 600 17	0	1	0
1	E	426	Total C N O S 3301 2111 577 596 17	0	1	0
1	F	425	Total C H N O S 3302 2112 1 578 594 17	0	1	0
1	G	425	Total C H N O S 3286 2102 2 574 591 17	0	0	0
1	H	425	Total C N O S 3282 2101 578 586 17	0	0	0
1	I	426	Total C N O S 3320 2121 585 597 17	0	1	0
1	J	425	Total C N O S 3298 2111 578 592 17	0	1	0
1	K	426	Total C N O S 3292 2106 576 593 17	0	0	0
1	L	425	Total C H N O S 3277 2098 1 575 586 17	0	0	0

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0

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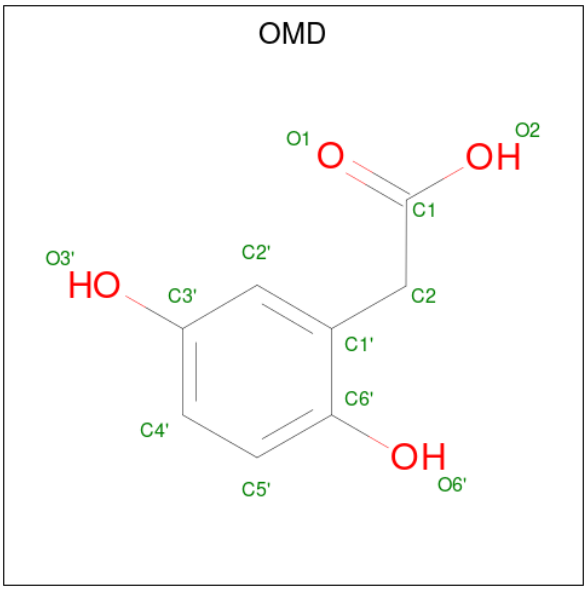
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe			
2	C	1	1	1		0	0
2	D	1	1	1		0	0
2	E	1	1	1		0	0
2	F	1	1	1		0	0
2	G	1	1	1		0	0
2	H	1	1	1		0	0
2	I	1	1	1		0	0
2	J	1	1	1		0	0
2	K	1	1	1		0	0
2	L	1	1	1		0	0

- Molecule 3 is 2-(3,6-DIHYDROXYPHENYL)ACETIC ACID (three-letter code: OMD) (formula: $C_8H_8O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	12	8	4	0	0

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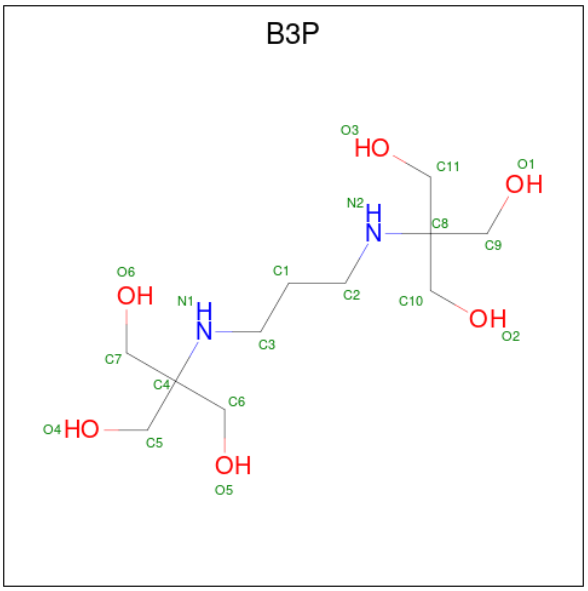
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	B	1	12	8	4		0	0
3	C	1	12	8	4		0	0
3	D	1	12	8	4		0	0
3	E	1	12	8	4		0	0
3	F	1	12	8	4		0	0
3	G	1	12	8	4		0	0
3	H	1	12	8	4		0	0
3	I	1	12	8	4		0	0
3	J	1	12	8	4		0	0
3	K	1	12	8	4		0	0
3	L	1	12	8	4		0	0

- Molecule 4 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	K	1	41	11	22	2	6	0	0

- Molecule 5 is water.

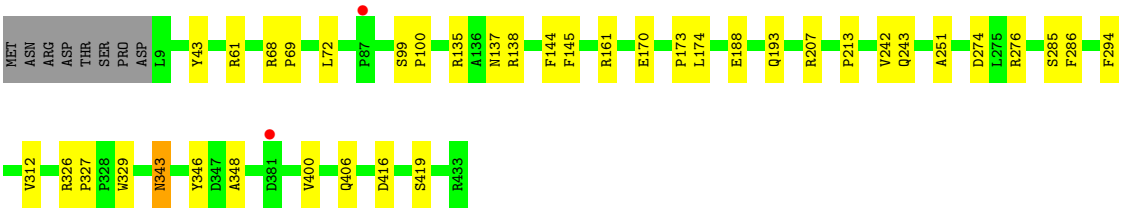
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	482	488	488	0	6
5	B	424	425	425	0	1
5	C	377	384	384	0	7
5	D	439	441	441	0	2
5	E	398	401	401	0	3
5	F	333	336	336	0	3
5	G	378	379	379	0	1
5	H	365	369	369	0	4
5	I	338	340	340	0	2
5	J	350	352	352	0	2
5	K	368	368	368	0	0
5	L	328	329	329	0	1

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.

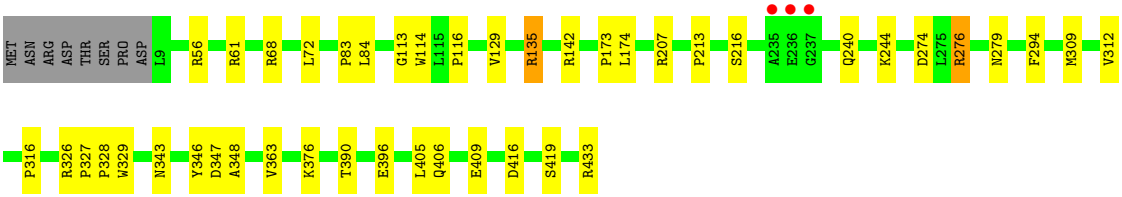
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain A:



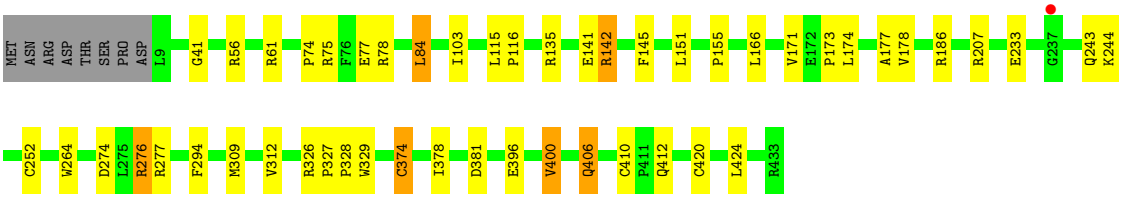
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain B:



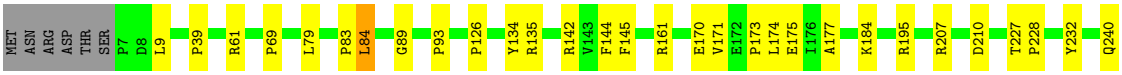
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain C:



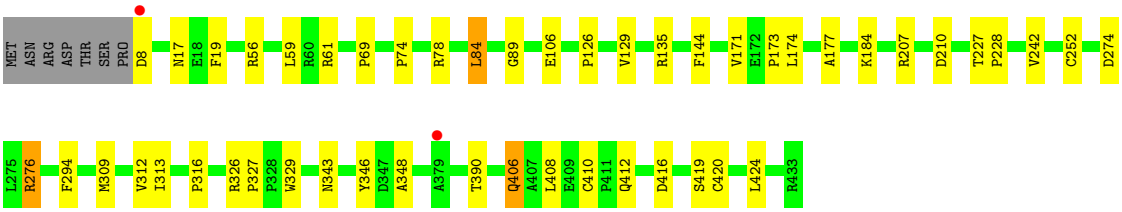
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain D:



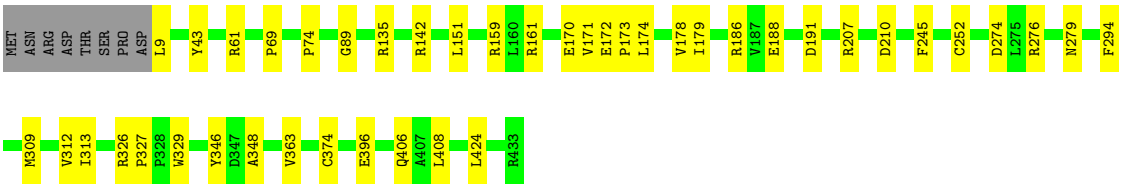
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain E:



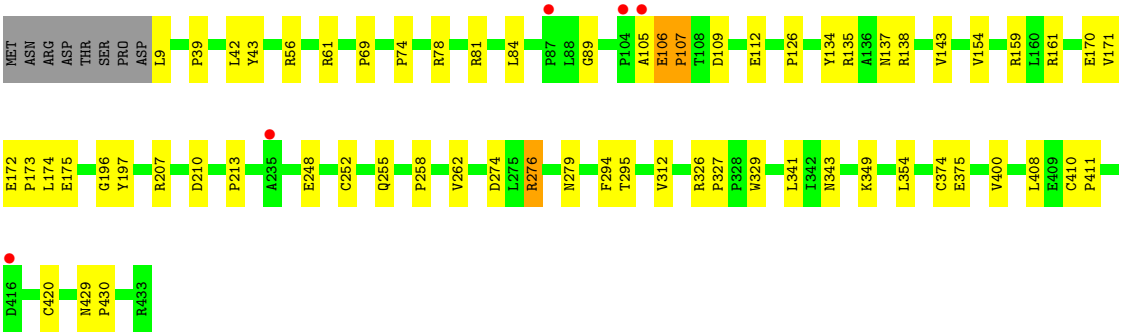
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain F:



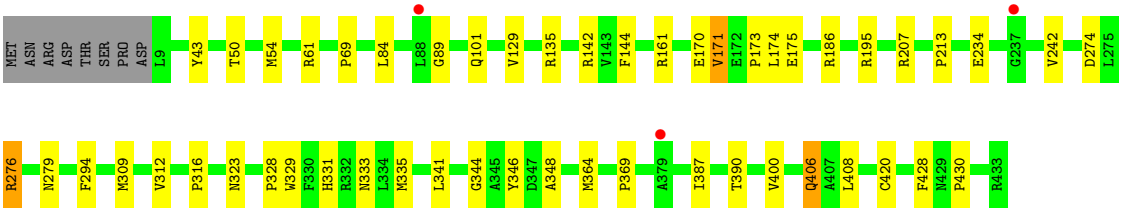
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain G:



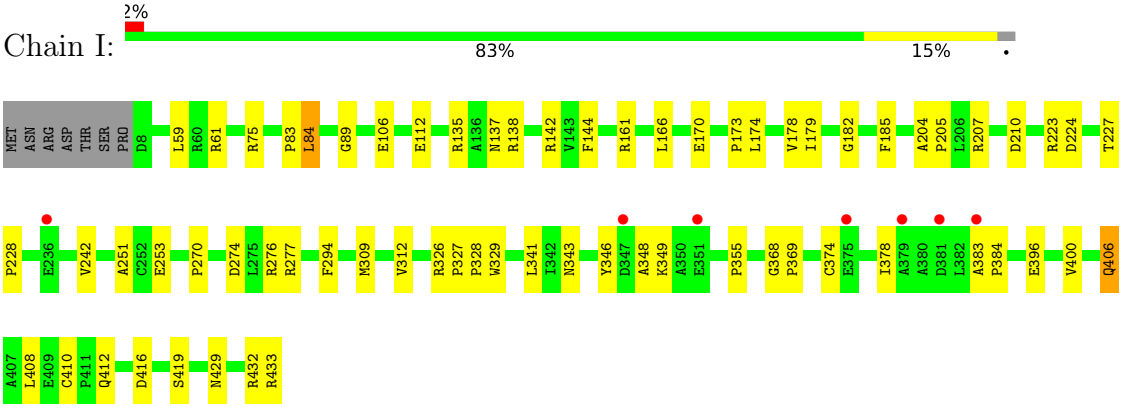
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain H:



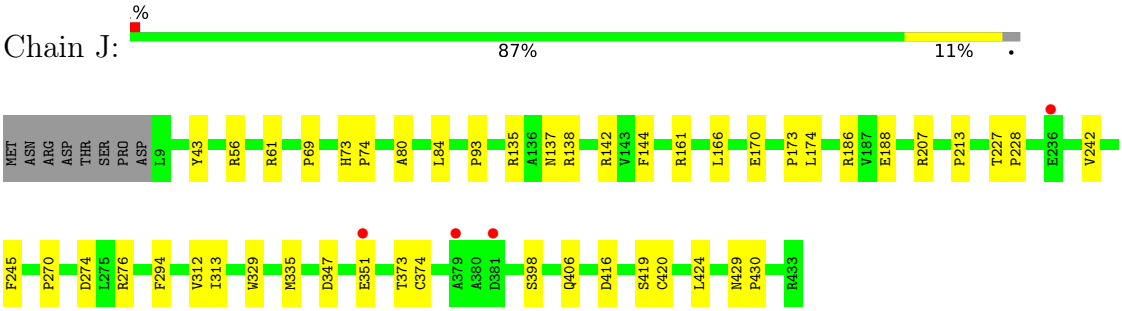
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain I:



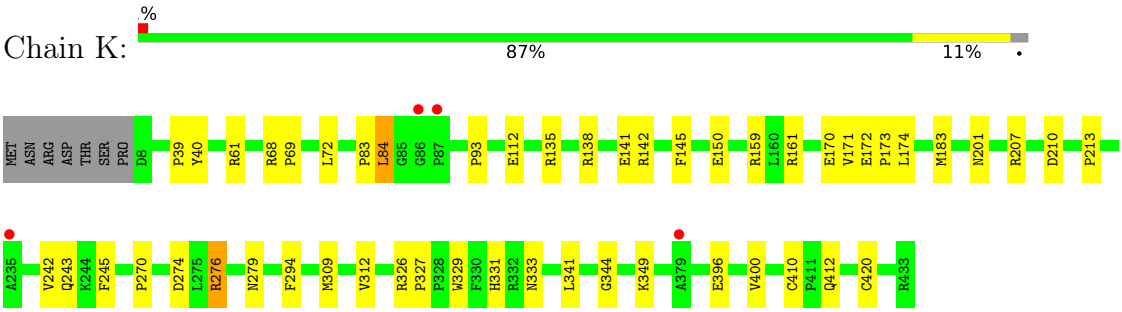
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain J:



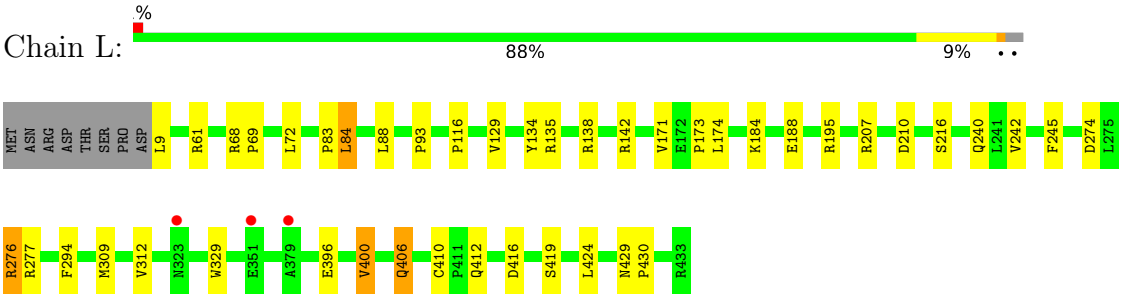
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain K:



• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	93.39Å 93.71Å 162.98Å 87.69° 80.42° 68.39°	Depositor
Resolution (Å)	34.17 – 1.98 34.17 – 1.98	Depositor EDS
% Data completeness (in resolution range)	95.6 (34.17-1.98) 95.6 (34.17-1.98)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 1.98Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.161 , 0.216 0.160 , 0.214	Depositor DCC
R_{free} test set	16870 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	44389	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: B3P, OMD, FE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.39	0/3411	0.55	0/4653
1	B	0.38	0/3401	0.53	0/4640
1	C	0.38	0/3399	0.54	0/4637
1	D	0.39	0/3416	0.55	0/4662
1	E	0.39	0/3403	0.55	0/4645
1	F	0.39	0/3403	0.54	0/4643
1	G	0.34	0/3385	0.51	0/4620
1	H	0.35	0/3384	0.51	0/4619
1	I	0.35	0/3422	0.51	0/4667
1	J	0.34	0/3400	0.51	0/4639
1	K	0.36	0/3394	0.53	0/4633
1	L	0.37	0/3378	0.53	0/4612
All	All	0.37	0/40796	0.53	0/55670

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	3309	2	3196	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3300	0	3182	30	0
1	C	3298	0	3180	32	0
1	D	3313	0	3187	32	0
1	E	3301	0	3174	34	0
1	F	3301	1	3187	23	0
1	G	3284	2	3159	49	0
1	H	3282	0	3168	33	0
1	I	3320	0	3211	48	0
1	J	3298	0	3185	26	0
1	K	3292	0	3169	28	0
1	L	3276	1	3157	34	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	12	0	6	0	0
3	B	12	0	6	0	0
3	C	12	0	6	1	0
3	D	12	0	6	1	0
3	E	12	0	6	0	0
3	F	12	0	6	0	0
3	G	12	0	6	0	0
3	H	12	0	6	1	0
3	I	12	0	6	0	0
3	J	12	0	6	0	0
3	K	12	0	6	0	0
3	L	12	0	6	0	0
4	K	19	22	25	1	0
5	A	488	0	0	2	0
5	B	425	0	0	9	2
5	C	384	0	0	5	1
5	D	441	0	0	9	0
5	E	401	0	0	6	0
5	F	336	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	379	0	0	7	0
5	H	369	0	0	7	0
5	I	340	0	0	8	0
5	J	352	0	0	5	1
5	K	368	0	0	2	0
5	L	329	0	0	4	0
All	All	44361	28	38252	372	2

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 5.

All (372) 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:56:ARG:CB	1:C:56:ARG:CD	2.48	0.91
1:B:56:ARG:CD	1:B:56:ARG:CB	2.50	0.90
1:G:56:ARG:CD	1:G:56:ARG:CB	2.51	0.88
1:G:106:GLU:HB3	1:G:107:PRO:HD3	1.55	0.87
1:G:106:GLU:CB	1:G:107:PRO:HD3	2.05	0.85
1:L:9:LEU:N	5:L:2003:HOH:O	2.10	0.83
1:G:56:ARG:NH2	5:G:2085:HOH:O	1.97	0.83
1:G:105:ALA:HB1	1:G:106:GLU:HG2	1.61	0.82
1:G:294:PHE:HB2	1:G:312:VAL:HG13	1.62	0.82
1:F:274:ASP:OD1	1:F:276:ARG:HD3	1.82	0.80
1:A:274:ASP:OD1	1:A:276:ARG:HD3	1.85	0.75
1:H:428:PHE:CE2	1:H:430:PRO:HG3	2.21	0.75
1:G:105:ALA:CB	1:G:106:GLU:HG2	2.17	0.74
1:E:106:GLU:OE1	1:E:106:GLU:N	2.17	0.73
1:F:89:GLY:HA3	1:F:408:LEU:HD12	1.70	0.72
1:J:161:ARG:NH1	1:J:170:GLU:OE2	2.22	0.72
1:G:106:GLU:CB	1:G:107:PRO:CD	2.65	0.72
1:E:410:CYS:SG	1:E:412:GLN:HB2	2.30	0.71
1:D:343:ASN:C	1:D:343:ASN:HD22	1.93	0.71
1:L:294:PHE:HB2	1:L:312:VAL:HG13	1.71	0.71
1:C:294:PHE:HB2	1:C:312:VAL:HG13	1.72	0.70
1:B:405:LEU:O	1:B:409:GLU:HG3	1.92	0.70
1:E:406[A]:GLN:H	1:E:406[A]:GLN:NE2	1.89	0.70
1:K:161:ARG:NH1	1:K:170:GLU:OE2	2.25	0.70
1:I:106:GLU:CD	1:I:106:GLU:H	1.96	0.69
1:H:89:GLY:HA3	1:H:408:LEU:HD12	1.75	0.69
1:B:294:PHE:HB2	1:B:312:VAL:HG13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ASP:OD1	1:C:276:ARG:HD3	1.93	0.67
1:L:138:ARG:HH11	1:L:138:ARG:HG2	1.59	0.67
1:A:193:GLN:HG3	5:A:2283:HOH:O	1.95	0.67
1:G:39:PRO:HD2	5:G:2037:HOH:O	1.95	0.66
1:B:347:ASP:OD2	5:B:2343:HOH:O	2.12	0.66
1:G:81:ARG:CZ	1:G:112:GLU:HG2	2.25	0.66
1:L:188:GLU:OE1	5:L:2182:HOH:O	2.11	0.66
1:E:126:PRO:HA	5:E:2184:HOH:O	1.95	0.66
1:G:106:GLU:HB3	1:G:107:PRO:CD	2.20	0.66
1:F:174:LEU:HB3	1:F:276:ARG:HD2	1.78	0.65
1:H:274:ASP:OD1	1:H:276:ARG:HD3	1.95	0.65
1:K:274:ASP:OD1	1:K:276:ARG:HD3	1.95	0.65
1:E:274:ASP:OD1	1:E:276:ARG:HD3	1.96	0.65
1:L:142:ARG:HD2	1:L:242:VAL:HG21	1.78	0.65
1:I:173:PRO:O	1:I:174:LEU:HB2	1.97	0.65
1:I:253:GLU:HB2	5:I:2246:HOH:O	1.97	0.64
1:G:9:LEU:CD1	1:G:170:GLU:HG3	2.28	0.64
1:J:351:GLU:HA	5:J:2305:HOH:O	1.99	0.63
1:G:159:ARG:HG2	1:G:172:GLU:HB3	1.80	0.63
1:I:294:PHE:HB2	1:I:312:VAL:HG13	1.79	0.63
1:K:138:ARG:HD2	5:K:2183:HOH:O	1.98	0.63
1:K:83:PRO:HB2	1:K:84:LEU:HD13	1.80	0.63
1:K:150:GLU:HB3	1:K:201:ASN:HB3	1.81	0.62
1:H:428:PHE:CZ	1:H:430:PRO:HG3	2.34	0.62
1:G:105:ALA:CA	1:G:106:GLU:HG2	2.30	0.61
1:L:142:ARG:HD2	1:L:242:VAL:CG2	2.31	0.61
1:I:274:ASP:OD1	1:I:276:ARG:HD3	2.01	0.61
1:K:274:ASP:OD1	1:K:276:ARG:CD	2.49	0.60
1:B:416:ASP:OD1	1:B:419:SER:HB3	2.01	0.60
1:D:145:PHE:HB3	1:D:184:LYS:HG3	1.82	0.60
1:I:416:ASP:OD2	1:I:419:SER:HB3	2.01	0.60
1:D:184:LYS:HD2	5:D:2265:HOH:O	2.02	0.60
1:H:173:PRO:O	1:H:174:LEU:HB2	2.01	0.60
1:B:142:ARG:HD3	1:B:240:GLN:OE1	2.02	0.60
1:K:69:PRO:HG2	1:L:424:LEU:HD13	1.82	0.59
1:J:347:ASP:OD2	5:J:2273:HOH:O	2.16	0.59
1:A:416:ASP:OD2	1:A:419:SER:HB3	2.02	0.59
1:A:69:PRO:HG2	1:C:424:LEU:HD13	1.85	0.58
1:J:173:PRO:O	1:J:174:LEU:HB2	2.03	0.58
1:B:274:ASP:OD1	1:B:276:ARG:HD2	2.04	0.58
1:G:89:GLY:HA3	1:G:408:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:LEU:HD11	1:G:170:GLU:HG3	1.86	0.58
1:H:341:LEU:HD21	1:H:344:GLY:O	2.04	0.58
1:B:83:PRO:HB2	1:B:84:LEU:HD13	1.85	0.58
1:D:171:VAL:HG21	1:D:177:ALA:HB2	1.85	0.58
1:L:274:ASP:OD1	1:L:276:ARG:HD3	2.03	0.58
1:D:343:ASN:C	1:D:343:ASN:ND2	2.56	0.57
1:G:106:GLU:HB2	1:G:107:PRO:HD3	1.86	0.57
1:E:106:GLU:H	1:E:106:GLU:CD	2.07	0.57
1:D:274:ASP:OD1	1:D:276:ARG:HD3	2.05	0.56
1:G:274:ASP:OD1	1:G:276:ARG:HD3	2.03	0.56
1:H:101:GLN:O	1:H:195:ARG:NH1	2.36	0.56
1:C:328:PRO:HB3	3:C:838:OMD:C4'	2.35	0.56
1:G:173:PRO:O	1:G:174:LEU:HB2	2.05	0.56
1:L:274:ASP:OD1	1:L:276:ARG:CD	2.53	0.56
1:A:174:LEU:HB3	1:A:276:ARG:HD2	1.86	0.56
1:E:84:LEU:O	5:E:2130:HOH:O	2.18	0.56
1:G:143:VAL:HG21	1:G:258:PRO:HG2	1.87	0.56
1:F:406[A]:GLN:CD	1:F:406[A]:GLN:H	2.09	0.56
1:C:74:PRO:HG2	1:C:252:CYS:HB2	1.88	0.56
1:H:406:GLN:CD	1:H:406:GLN:H	2.10	0.55
1:J:43:TYR:CD2	1:J:69:PRO:HD3	2.41	0.55
1:E:346:TYR:CE2	1:E:348:ALA:HB3	2.41	0.55
1:H:161:ARG:HD2	1:H:170:GLU:OE2	2.06	0.55
1:C:173:PRO:O	1:C:174:LEU:HB2	2.07	0.55
1:D:173:PRO:O	1:D:174:LEU:HB2	2.07	0.55
1:A:294:PHE:HB2	1:A:312:VAL:HG13	1.88	0.55
1:C:374:CYS:O	1:C:378:ILE:HG13	2.07	0.55
1:J:161:ARG:HD3	1:J:188:GLU:OE1	2.06	0.54
1:G:126:PRO:HA	5:G:2171:HOH:O	2.07	0.54
1:K:410:CYS:SG	1:K:412:GLN:HB2	2.48	0.54
1:D:84:LEU:HD23	1:D:244:LYS:HE2	1.90	0.54
1:I:326:ARG:N	1:I:327:PRO:CD	2.70	0.54
1:D:89:GLY:HA3	1:D:408:LEU:HD12	1.88	0.54
1:A:173:PRO:O	1:A:174:LEU:HB2	2.07	0.54
1:B:346:TYR:CE2	1:B:348:ALA:HB3	2.43	0.54
1:J:294:PHE:HB2	1:J:312:VAL:HG13	1.90	0.54
5:B:2247:HOH:O	1:E:56:ARG:HB2	2.08	0.54
1:I:89:GLY:HA3	1:I:408:LEU:HD12	1.89	0.54
1:K:159:ARG:HG2	1:K:172:GLU:HB3	1.90	0.54
1:B:406[B]:GLN:NE2	5:B:2126:HOH:O	2.41	0.53
1:D:171:VAL:HG13	1:D:175:GLU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:2125:HOH:O	1:I:75:ARG:NH1	2.40	0.53
1:I:429:ASN:ND2	5:I:2337:HOH:O	2.41	0.53
1:A:161:ARG:NH1	1:A:170:GLU:OE2	2.39	0.53
1:B:406[A]:GLN:H	1:B:406[A]:GLN:NE2	2.07	0.53
1:F:346:TYR:CE2	1:F:348:ALA:HB3	2.44	0.53
1:G:105:ALA:HA	1:G:106:GLU:CG	2.38	0.53
1:C:155:PRO:HG2	1:C:171:VAL:HG12	1.91	0.53
1:D:346:TYR:CE2	1:D:348:ALA:HB3	2.44	0.53
1:I:161:ARG:NH1	1:I:170:GLU:OE2	2.39	0.52
1:B:274:ASP:OD1	1:B:276:ARG:CD	2.57	0.52
1:E:173:PRO:O	1:E:174:LEU:HB2	2.07	0.52
1:C:277:ARG:NE	5:C:2280:HOH:O	2.32	0.52
1:D:210:ASP:CB	5:D:2280:HOH:O	2.58	0.52
1:D:227:THR:HG23	1:D:228:PRO:HD2	1.91	0.52
1:D:134:TYR:O	1:D:195:ARG:HA	2.08	0.52
1:L:173:PRO:O	1:L:174:LEU:HB2	2.10	0.52
1:A:326:ARG:N	1:A:327:PRO:CD	2.73	0.52
1:D:274:ASP:OD1	1:D:276:ARG:CD	2.57	0.52
1:H:234:GLU:OE2	5:H:2247:HOH:O	2.18	0.52
1:I:346:TYR:CE2	1:I:348:ALA:HB3	2.45	0.52
1:I:227:THR:HG23	1:I:228:PRO:HD2	1.91	0.52
1:G:408:LEU:O	5:G:2368:HOH:O	2.19	0.52
1:D:328:PRO:HB3	3:D:838:OMD:C4'	2.39	0.52
1:G:105:ALA:HA	1:G:106:GLU:HG2	1.91	0.52
1:I:84:LEU:N	1:I:84:LEU:CD1	2.73	0.52
1:I:174:LEU:HB3	1:I:276:ARG:HD2	1.91	0.52
1:A:161:ARG:HB3	1:A:188:GLU:HB3	1.93	0.51
1:C:141:GLU:O	1:C:142:ARG:HB3	2.09	0.51
1:G:39:PRO:HA	1:I:433:ARG:OXT	2.10	0.51
1:K:173:PRO:O	1:K:174:LEU:HB2	2.10	0.51
1:K:245:PHE:CD2	1:L:93:PRO:HB3	2.45	0.51
1:I:224:ASP:OD1	1:I:277:ARG:NH1	2.43	0.51
1:D:9:LEU:HG	5:D:2002:HOH:O	2.10	0.51
1:H:213:PRO:HD3	1:L:210:ASP:O	2.09	0.51
1:F:309:MET:HA	1:F:396:GLU:O	2.10	0.51
1:H:144:PHE:HA	1:H:242:VAL:O	2.10	0.51
1:C:171:VAL:HG21	1:C:177:ALA:HB2	1.93	0.51
1:D:126:PRO:HA	5:D:2197:HOH:O	2.11	0.51
1:D:161:ARG:NH1	1:D:170:GLU:OE2	2.37	0.51
1:D:416:ASP:HA	5:D:2426:HOH:O	2.11	0.51
1:D:93:PRO:HB3	1:F:245:PHE:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:223:ARG:HD2	5:I:2232:HOH:O	2.10	0.51
1:E:174:LEU:HD21	1:E:343:ASN:ND2	2.26	0.50
5:K:2078:HOH:O	1:L:400:VAL:HG22	2.10	0.50
1:C:75:ARG:NH1	1:C:77:GLU:HG2	2.26	0.50
1:L:142:ARG:HD3	1:L:240:GLN:OE1	2.11	0.50
1:L:68:ARG:HD3	1:L:72:LEU:HD23	1.94	0.50
1:J:227:THR:HG23	1:J:228:PRO:HD2	1.93	0.50
1:G:74:PRO:HG2	1:G:252:CYS:HB2	1.93	0.50
1:B:216:SER:HB2	1:E:59:LEU:HD21	1.94	0.50
1:H:328:PRO:HB3	3:H:838:OMD:C4'	2.41	0.50
1:G:81:ARG:NE	1:G:112:GLU:HG2	2.27	0.49
1:G:341:LEU:HD23	1:G:354:LEU:C	2.32	0.49
1:D:326:ARG:N	1:D:327:PRO:CD	2.75	0.49
1:L:83:PRO:HG2	1:L:84:LEU:HD22	1.93	0.49
1:D:39:PRO:HD2	5:D:2042:HOH:O	2.12	0.49
1:E:294:PHE:HB3	1:E:313:ILE:O	2.13	0.49
1:H:364:MET:HG3	1:I:182:GLY:CA	2.43	0.49
1:G:78:ARG:HE	1:G:248:GLU:CD	2.15	0.49
1:K:294:PHE:HB2	1:K:312:VAL:HG13	1.95	0.49
1:L:84:LEU:HD12	1:L:116:PRO:HG3	1.95	0.49
1:A:400:VAL:CG2	5:A:2106:HOH:O	2.61	0.49
1:B:129:VAL:HG21	1:B:309:MET:HB3	1.93	0.49
1:F:161:ARG:HB3	1:F:188:GLU:HB3	1.94	0.49
1:D:83:PRO:HB2	1:D:84:LEU:HD13	1.94	0.49
1:C:41:GLY:HA2	5:C:2062:HOH:O	2.13	0.48
1:K:142:ARG:HD2	1:K:242:VAL:HG21	1.94	0.48
1:K:326:ARG:N	1:K:327:PRO:CD	2.76	0.48
1:B:213:PRO:HD3	1:F:210:ASP:O	2.14	0.48
1:I:309:MET:HA	1:I:396:GLU:O	2.12	0.48
1:H:328:PRO:O	1:H:369:PRO:HD3	2.13	0.48
1:I:368:GLY:HA2	5:I:2285:HOH:O	2.13	0.48
1:L:309:MET:HA	1:L:396:GLU:O	2.13	0.48
1:B:173:PRO:O	1:B:174:LEU:HB2	2.14	0.48
1:H:171:VAL:HG12	1:H:175:GLU:CB	2.44	0.48
1:H:364:MET:HG3	1:I:182:GLY:HA3	1.96	0.48
1:A:343:ASN:C	1:A:343:ASN:ND2	2.67	0.48
1:E:227:THR:HG23	1:E:228:PRO:HD2	1.96	0.47
1:I:406[A]:GLN:HG3	5:I:2324:HOH:O	2.12	0.47
1:L:138:ARG:HG2	1:L:138:ARG:NH1	2.27	0.47
1:C:84:LEU:HD23	1:C:244:LYS:HE2	1.96	0.47
1:E:69:PRO:HG2	1:F:424:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:PRO:HG2	1:E:424:LEU:HD13	1.96	0.47
1:E:294:PHE:HB2	1:E:312:VAL:HG13	1.95	0.47
1:F:9:LEU:CD1	1:F:170:GLU:HG3	2.45	0.47
1:F:74:PRO:HG2	1:F:252:CYS:HB2	1.97	0.47
1:H:142:ARG:O	1:H:186:ARG:HG3	2.14	0.47
1:G:213:PRO:HD3	1:K:210:ASP:O	2.15	0.47
1:I:341:LEU:O	1:I:355:PRO:HA	2.14	0.47
1:E:78:ARG:NH1	5:E:2114:HOH:O	2.24	0.47
1:J:80:ALA:O	5:J:2101:HOH:O	2.20	0.47
1:C:309:MET:HA	1:C:396:GLU:O	2.15	0.47
1:G:137:ASN:OD1	1:G:138:ARG:HG2	2.15	0.47
1:D:210:ASP:CB	5:D:2281:HOH:O	2.62	0.47
1:F:173:PRO:O	1:F:174:LEU:HB2	2.15	0.47
1:G:105:ALA:HA	1:G:106:GLU:HA	1.46	0.46
1:H:173:PRO:O	1:H:174:LEU:CB	2.63	0.46
1:H:294:PHE:HB2	1:H:312:VAL:HG13	1.96	0.46
1:B:316:PRO:HD3	1:B:390:THR:O	2.14	0.46
1:C:274:ASP:OD1	1:C:276:ARG:CD	2.63	0.46
1:F:294:PHE:HB2	1:F:312:VAL:HG13	1.97	0.46
1:I:59:LEU:HD21	1:L:216:SER:HB2	1.97	0.46
1:G:43:TYR:CD2	1:G:69:PRO:HD3	2.50	0.46
1:G:210:ASP:O	1:K:213:PRO:HD3	2.14	0.46
1:I:410:CYS:SG	1:I:412:GLN:OE1	2.73	0.46
5:B:2069:HOH:O	1:C:78:ARG:HD2	2.16	0.46
1:A:43:TYR:CD1	1:A:69:PRO:HD3	2.50	0.46
1:F:142:ARG:O	1:F:186:ARG:HG3	2.15	0.46
1:G:161:ARG:HG3	1:G:170:GLU:HG2	1.97	0.46
1:I:174:LEU:HD13	1:I:276:ARG:HD2	1.98	0.46
1:B:343:ASN:C	1:B:343:ASN:OD1	2.53	0.46
1:J:424:LEU:HD13	1:L:69:PRO:HG2	1.96	0.46
1:E:171:VAL:HG21	1:E:177:ALA:HB2	1.98	0.46
5:H:2062:HOH:O	1:I:75:ARG:HD2	2.16	0.46
1:E:406[A]:GLN:H	1:E:406[A]:GLN:HE21	1.62	0.45
1:C:142:ARG:O	1:C:186:ARG:HG3	2.16	0.45
1:C:406:GLN:CD	1:C:406:GLN:H	2.19	0.45
1:F:89:GLY:HA3	1:F:408:LEU:CD1	2.45	0.45
1:C:410:CYS:SG	1:C:412:GLN:HB2	2.57	0.45
1:I:83:PRO:HB2	1:I:84:LEU:HD13	1.98	0.45
1:J:373:THR:HG23	5:J:2303:HOH:O	2.16	0.45
1:B:68:ARG:HD3	1:B:72:LEU:HD23	1.98	0.45
1:J:137:ASN:OD1	1:J:138:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:ARG:N	1:C:327:PRO:CD	2.80	0.45
1:E:89:GLY:HA3	1:E:408:LEU:HD12	1.99	0.45
1:A:213:PRO:HD3	1:E:210:ASP:O	2.17	0.45
1:B:84:LEU:HD23	1:B:244:LYS:HE2	1.99	0.45
1:H:406:GLN:HG3	5:H:2354:HOH:O	2.17	0.45
1:H:43:TYR:CD2	1:H:69:PRO:HG3	2.52	0.45
1:E:144:PHE:HA	1:E:242:VAL:O	2.16	0.44
1:K:39:PRO:O	1:K:40:TYR:HB2	2.15	0.44
1:E:8:ASP:N	5:E:2001:HOH:O	2.50	0.44
1:G:174:LEU:HD13	1:G:276:ARG:HE	1.82	0.44
1:G:255:GLN:NE2	5:G:2269:HOH:O	2.46	0.44
1:H:171:VAL:HG12	1:H:175:GLU:HB2	1.99	0.44
1:J:294:PHE:HB3	1:J:313:ILE:O	2.17	0.44
1:L:294:PHE:CB	1:L:312:VAL:HG13	2.45	0.44
1:G:161:ARG:HD2	1:G:170:GLU:OE2	2.18	0.44
1:I:406[A]:GLN:CD	1:I:406[A]:GLN:H	2.21	0.44
1:D:142:ARG:HD3	1:D:240:GLN:OE1	2.17	0.44
1:L:410:CYS:SG	1:L:412:GLN:HB2	2.57	0.44
1:J:144:PHE:HA	1:J:242:VAL:O	2.17	0.44
1:A:69:PRO:CG	1:C:424:LEU:HD13	2.46	0.44
1:D:377:ALA:HA	5:D:2400:HOH:O	2.18	0.44
1:F:159:ARG:HG2	1:F:172:GLU:HB3	2.00	0.44
1:G:42:LEU:HD21	1:G:262:VAL:HG21	1.99	0.44
1:L:406:GLN:HG3	5:L:2312:HOH:O	2.18	0.44
1:E:129:VAL:HG21	1:E:309:MET:HB3	2.00	0.43
1:F:178:VAL:O	1:F:179:ILE:HD13	2.18	0.43
1:C:400:VAL:HG13	5:C:2355:HOH:O	2.17	0.43
1:G:134:TYR:CZ	1:G:196:GLY:HA3	2.53	0.43
1:I:144:PHE:HA	1:I:242:VAL:O	2.18	0.43
1:H:400:VAL:CG2	5:H:2072:HOH:O	2.66	0.43
1:L:274:ASP:OD1	1:L:276:ARG:HD2	2.19	0.43
1:F:159:ARG:NH2	1:F:191:ASP:OD1	2.34	0.43
1:I:210:ASP:O	1:J:213:PRO:HD3	2.19	0.43
1:I:223:ARG:NH2	5:I:2235:HOH:O	2.51	0.43
1:E:416:ASP:HA	5:E:2390:HOH:O	2.18	0.43
5:G:2227:HOH:O	1:J:56:ARG:NH2	2.25	0.43
1:I:84:LEU:N	1:I:84:LEU:HD13	2.33	0.43
1:I:166:LEU:HD12	1:I:270:PRO:HD2	2.00	0.43
1:C:233:GLU:HG2	5:C:2269:HOH:O	2.18	0.43
1:J:166:LEU:HD12	1:J:270:PRO:HD2	2.00	0.43
1:L:429:ASN:HA	1:L:430:PRO:HD2	1.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ARG:N	1:B:327:PRO:CD	2.82	0.43
1:C:103:ILE:HD11	5:C:2201:HOH:O	2.18	0.43
1:I:432:ARG:NH1	5:I:2339:HOH:O	2.30	0.43
1:B:294:PHE:HB2	1:B:312:VAL:CG1	2.46	0.43
1:J:416:ASP:OD2	1:J:419:SER:HB3	2.18	0.43
1:I:400:VAL:HG13	5:I:2320:HOH:O	2.19	0.43
1:K:349:LYS:HD3	1:K:349:LYS:HA	1.85	0.43
1:L:406:GLN:H	1:L:406:GLN:CD	2.22	0.43
1:C:75:ARG:HH12	1:C:77:GLU:HG2	1.83	0.42
1:C:145:PHE:O	1:C:243:GLN:HA	2.18	0.42
1:D:79:LEU:HD21	1:D:251:ALA:HB3	2.00	0.42
1:E:74:PRO:HG2	1:E:252:CYS:HB2	2.00	0.42
1:K:145:PHE:O	1:K:243:GLN:HA	2.18	0.42
1:A:144:PHE:HA	1:A:242:VAL:O	2.19	0.42
1:I:173:PRO:O	1:I:174:LEU:CB	2.66	0.42
1:J:335:MET:HE1	1:J:398:SER:HB3	2.01	0.42
1:K:331:HIS:CE1	1:K:333:ASN:HB2	2.54	0.42
1:A:137:ASN:O	1:A:138:ARG:HD3	2.19	0.42
1:A:346:TYR:CE2	1:A:348:ALA:HB3	2.55	0.42
1:K:309:MET:HA	1:K:396:GLU:O	2.19	0.42
5:G:2036:HOH:O	1:I:433:ARG:NH1	2.46	0.42
1:H:129:VAL:HG21	1:H:309:MET:HB3	2.02	0.42
1:K:141:GLU:OE1	4:K:1436:B3P:N2	2.53	0.42
1:D:406[A]:GLN:HG3	5:D:2417:HOH:O	2.19	0.42
1:G:295:THR:HA	1:G:312:VAL:HG22	2.01	0.42
1:K:68:ARG:HD3	1:K:72:LEU:HD23	2.02	0.42
1:K:183:MET:SD	1:K:270:PRO:HD3	2.60	0.42
1:L:277:ARG:CZ	5:L:2234:HOH:O	2.68	0.42
1:B:309:MET:HA	1:B:396:GLU:O	2.20	0.42
1:C:151:LEU:O	1:C:178:VAL:HA	2.20	0.42
1:I:137:ASN:OD1	1:I:138:ARG:HG2	2.19	0.42
1:I:374:CYS:O	1:I:378:ILE:HG13	2.19	0.42
1:J:93:PRO:HB3	1:L:245:PHE:CD2	2.54	0.42
1:L:88:LEU:HD23	1:L:88:LEU:HA	1.91	0.42
1:A:68:ARG:HD3	1:A:72:LEU:HD23	2.02	0.42
1:H:331:HIS:CE1	1:H:333:ASN:HB2	2.54	0.42
1:I:204:ALA:HA	1:I:205:PRO:HD3	1.92	0.42
1:L:129:VAL:HG21	1:L:309:MET:HB3	2.02	0.42
1:B:113:GLY:HA3	1:B:135:ARG:O	2.20	0.42
1:B:328:PRO:HG2	1:B:348:ALA:HB2	2.02	0.42
1:B:376:LYS:HB3	1:B:376:LYS:HE2	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:294:PHE:HB3	1:F:313:ILE:O	2.19	0.42
1:G:349:LYS:HA	1:G:349:LYS:HD3	1.85	0.42
1:J:245:PHE:CD2	1:K:93:PRO:HB3	2.55	0.42
1:L:416:ASP:OD1	1:L:419:SER:HB3	2.20	0.42
1:B:114:TRP:O	1:B:116:PRO:HD3	2.20	0.42
1:B:433:ARG:HD2	5:B:2424:HOH:O	2.19	0.42
1:G:326:ARG:N	1:G:327:PRO:CD	2.83	0.42
1:G:429:ASN:HA	1:G:430:PRO:HD2	1.89	0.42
1:H:316:PRO:HD3	1:H:390:THR:O	2.20	0.42
1:H:335:MET:HG3	5:H:2345:HOH:O	2.20	0.42
1:I:179:ILE:HG21	1:I:185:PHE:CD1	2.55	0.42
1:I:328:PRO:O	1:I:369:PRO:HD3	2.20	0.42
1:A:343:ASN:C	1:A:343:ASN:HD22	2.23	0.41
1:G:109:ASP:OD1	1:G:112:GLU:HB2	2.19	0.41
1:L:134:TYR:O	1:L:195:ARG:HA	2.20	0.41
1:I:112:GLU:OE2	1:I:142:ARG:NH2	2.52	0.41
1:A:285:SER:OG	1:A:286:PHE:N	2.53	0.41
1:C:115:LEU:HD12	1:C:116:PRO:HD2	2.02	0.41
1:E:326:ARG:N	1:E:327:PRO:CD	2.82	0.41
1:G:174:LEU:CD1	1:G:276:ARG:HE	2.34	0.41
1:B:406[A]:GLN:HG3	5:B:2397:HOH:O	2.20	0.41
1:E:17:ASN:HB2	1:E:19:PHE:CZ	2.55	0.41
1:E:184:LYS:HE3	5:E:2243:HOH:O	2.19	0.41
1:E:316:PRO:HD3	1:E:390:THR:O	2.20	0.41
1:E:416:ASP:OD2	1:E:419:SER:HB3	2.20	0.41
1:J:142:ARG:O	1:J:186:ARG:HG3	2.20	0.41
5:B:2083[B]:HOH:O	1:E:210:ASP:HB2	2.20	0.41
5:B:2248:HOH:O	1:E:56:ARG:NH2	2.28	0.41
1:J:274:ASP:OD1	1:J:276:ARG:HD3	2.20	0.41
5:J:2289:HOH:O	1:L:184:LYS:HE3	2.20	0.41
1:K:112:GLU:OE2	1:K:142:ARG:NH2	2.53	0.41
1:D:144:PHE:O	1:D:184:LYS:HA	2.21	0.41
1:H:346:TYR:CE2	1:H:348:ALA:HB3	2.56	0.41
1:G:172:GLU:O	1:G:175:GLU:HB2	2.21	0.41
1:K:341:LEU:HD21	1:K:344:GLY:O	2.21	0.41
1:H:323:ASN:HB3	5:H:2299[A]:HOH:O	2.20	0.41
1:B:56:ARG:NH2	5:B:2086:HOH:O	2.35	0.41
1:C:166:LEU:HD13	1:C:264:TRP:CD2	2.56	0.41
1:F:326:ARG:N	1:F:327:PRO:CD	2.83	0.41
1:J:73:HIS:HA	1:J:74:PRO:HD3	1.82	0.41
1:J:429:ASN:HA	1:J:430:PRO:HD2	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:178:VAL:O	1:I:179:ILE:HD13	2.21	0.41
1:I:383:ALA:O	1:I:384:PRO:C	2.59	0.41
1:G:154:VAL:HB	1:G:197:TYR:HB2	2.03	0.40
1:J:43:TYR:CE2	1:J:69:PRO:HD3	2.56	0.40
1:G:410:CYS:HA	1:G:411:PRO:HD3	1.94	0.40
1:H:316:PRO:HA	1:H:387:ILE:O	2.21	0.40
1:F:43:TYR:CD2	1:F:69:PRO:HD3	2.56	0.40
1:A:242:VAL:HG22	1:A:251:ALA:HB2	2.03	0.40
1:A:99:SER:HB3	1:A:100:PRO:HD2	2.04	0.40
1:A:145:PHE:O	1:A:243:GLN:HA	2.21	0.40
1:C:141:GLU:O	1:C:142:ARG:CB	2.70	0.40
1:D:232:TYR:CD1	1:D:262:VAL:HG22	2.57	0.40
1:F:151:LEU:O	1:F:178:VAL:HA	2.21	0.40
1:H:50:THR:HB	1:H:54:MET:HG3	2.03	0.40
1:H:171:VAL:HG12	1:H:175:GLU:HB3	2.04	0.40
1:I:242:VAL:HG22	1:I:251:ALA:HB2	2.03	0.40
1:K:274:ASP:OD1	1:K:276:ARG:HD2	2.20	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2385:HOH:O	5:C:2379:HOH:O[1_565]	2.15	0.05
5:B:2401:HOH:O	5:J:2101:HOH:O[1_466]	2.16	0.04

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	424/433 (98%)	410 (97%)	14 (3%)	0	100 100
1	B	424/433 (98%)	411 (97%)	12 (3%)	1 (0%)	47 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	423/433 (98%)	408 (96%)	14 (3%)	1 (0%)	47	38
1	D	426/433 (98%)	414 (97%)	11 (3%)	1 (0%)	47	38
1	E	425/433 (98%)	414 (97%)	11 (3%)	0	100	100
1	F	424/433 (98%)	409 (96%)	14 (3%)	1 (0%)	47	38
1	G	423/433 (98%)	402 (95%)	19 (4%)	2 (0%)	29	16
1	H	423/433 (98%)	405 (96%)	18 (4%)	0	100	100
1	I	425/433 (98%)	410 (96%)	15 (4%)	0	100	100
1	J	424/433 (98%)	412 (97%)	12 (3%)	0	100	100
1	K	424/433 (98%)	412 (97%)	12 (3%)	0	100	100
1	L	423/433 (98%)	408 (96%)	15 (4%)	0	100	100
All	All	5088/5196 (98%)	4915 (97%)	167 (3%)	6 (0%)	51	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	106	GLU
1	C	142	ARG
1	G	107	PRO
1	B	363	VAL
1	D	363	VAL
1	F	363	VAL

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	342/355 (96%)	336 (98%)	6 (2%)	59	51
1	B	339/355 (96%)	333 (98%)	6 (2%)	59	51
1	C	340/355 (96%)	329 (97%)	11 (3%)	39	28
1	D	342/355 (96%)	331 (97%)	11 (3%)	39	28
1	E	339/355 (96%)	330 (97%)	9 (3%)	44	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	340/355 (96%)	333 (98%)	7 (2%)	53	47
1	G	336/355 (95%)	323 (96%)	13 (4%)	32	19
1	H	336/355 (95%)	326 (97%)	10 (3%)	41	29
1	I	343/355 (97%)	334 (97%)	9 (3%)	46	37
1	J	339/355 (96%)	330 (97%)	9 (3%)	44	35
1	K	338/355 (95%)	328 (97%)	10 (3%)	41	29
1	L	335/355 (94%)	326 (97%)	9 (3%)	44	35
All	All	4069/4260 (96%)	3959 (97%)	110 (3%)	46	35

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
1	A	135	ARG
1	A	207	ARG
1	A	329	TRP
1	A	343	ASN
1	A	406	GLN
1	B	61	ARG
1	B	135	ARG
1	B	207	ARG
1	B	276	ARG
1	B	279	ASN
1	B	329	TRP
1	C	61	ARG
1	C	84	LEU
1	C	135	ARG
1	C	207	ARG
1	C	276	ARG
1	C	329	TRP
1	C	374	CYS
1	C	381	ASP
1	C	400	VAL
1	C	406	GLN
1	C	420	CYS
1	D	61	ARG
1	D	84	LEU
1	D	135	ARG
1	D	207	ARG
1	D	276	ARG

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Mol	Chain	Res	Type
1	D	279	ASN
1	D	329	TRP
1	D	343	ASN
1	D	354	LEU
1	D	406[A]	GLN
1	D	406[B]	GLN
1	E	61	ARG
1	E	84	LEU
1	E	135	ARG
1	E	207	ARG
1	E	276	ARG
1	E	329	TRP
1	E	406[A]	GLN
1	E	406[B]	GLN
1	E	420	CYS
1	F	61	ARG
1	F	135	ARG
1	F	171	VAL
1	F	207	ARG
1	F	279	ASN
1	F	329	TRP
1	F	374	CYS
1	G	61	ARG
1	G	84	LEU
1	G	135	ARG
1	G	171	VAL
1	G	207	ARG
1	G	276	ARG
1	G	279	ASN
1	G	329	TRP
1	G	343	ASN
1	G	374	CYS
1	G	375	GLU
1	G	400	VAL
1	G	420	CYS
1	H	61	ARG
1	H	84	LEU
1	H	135	ARG
1	H	171	VAL
1	H	207	ARG
1	H	276	ARG
1	H	279	ASN

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Mol	Chain	Res	Type
1	H	329	TRP
1	H	406	GLN
1	H	420	CYS
1	I	61	ARG
1	I	84	LEU
1	I	135	ARG
1	I	207	ARG
1	I	329	TRP
1	I	343	ASN
1	I	349	LYS
1	I	406[A]	GLN
1	I	406[B]	GLN
1	J	61	ARG
1	J	84	LEU
1	J	135	ARG
1	J	207	ARG
1	J	329	TRP
1	J	374	CYS
1	J	406[A]	GLN
1	J	406[B]	GLN
1	J	420	CYS
1	K	61	ARG
1	K	84	LEU
1	K	135	ARG
1	K	171	VAL
1	K	207	ARG
1	K	276	ARG
1	K	279	ASN
1	K	329	TRP
1	K	400	VAL
1	K	420	CYS
1	L	61	ARG
1	L	84	LEU
1	L	135	ARG
1	L	171	VAL
1	L	207	ARG
1	L	276	ARG
1	L	329	TRP
1	L	400	VAL
1	L	406	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	231	HIS
1	A	343	ASN
1	B	231	HIS
1	C	193	GLN
1	D	343	ASN
1	E	343	ASN
1	G	101	GLN
1	H	304	HIS
1	H	399	GLN
1	I	429	ASN
1	J	101	GLN
1	K	304	HIS
1	L	343	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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)

Of 25 ligands modelled in this entry, 12 are monoatomic - leaving 13 for Mogul analysis.

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	$\#\|Z\| > 2$
3	OMD	J	838	2	12,12,12	0.76	0	16,16,16	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	OMD	F	838	2	12,12,12	0.83	0	16,16,16	0.83	0
3	OMD	B	838	2	12,12,12	0.63	0	16,16,16	0.84	0
3	OMD	E	838	2	12,12,12	0.79	0	16,16,16	1.02	1 (6%)
3	OMD	G	838	2	12,12,12	0.67	0	16,16,16	0.80	0
4	B3P	K	1436	-	18,18,18	1.28	3 (16%)	21,23,23	0.87	0
3	OMD	I	838	2	12,12,12	0.67	0	16,16,16	0.69	0
3	OMD	K	838	2	12,12,12	0.65	0	16,16,16	0.87	0
3	OMD	H	838	2	12,12,12	0.77	0	16,16,16	0.87	0
3	OMD	D	838	2	12,12,12	0.81	0	16,16,16	0.83	0
3	OMD	L	838	2	12,12,12	0.78	0	16,16,16	1.05	1 (6%)
3	OMD	C	838	2	12,12,12	0.83	0	16,16,16	1.00	1 (6%)
3	OMD	A	838	2	12,12,12	0.86	0	16,16,16	1.12	2 (12%)

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
3	OMD	J	838	2	-	0/4/4/4	0/1/1/1
3	OMD	F	838	2	-	0/4/4/4	0/1/1/1
3	OMD	B	838	2	-	0/4/4/4	0/1/1/1
3	OMD	E	838	2	-	0/4/4/4	0/1/1/1
3	OMD	G	838	2	-	0/4/4/4	0/1/1/1
4	B3P	K	1436	-	-	4/28/28/28	-
3	OMD	I	838	2	-	0/4/4/4	0/1/1/1
3	OMD	K	838	2	-	0/4/4/4	0/1/1/1
3	OMD	H	838	2	-	0/4/4/4	0/1/1/1
3	OMD	D	838	2	-	0/4/4/4	0/1/1/1
3	OMD	L	838	2	-	0/4/4/4	0/1/1/1
3	OMD	C	838	2	-	0/4/4/4	0/1/1/1
3	OMD	A	838	2	-	0/4/4/4	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1436	B3P	C2-N2	3.23	1.50	1.46
4	K	1436	B3P	C7-C4	2.50	1.56	1.53
4	K	1436	B3P	O3-C11	-2.02	1.35	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	838	OMD	C2-C1'-C6'	-2.35	118.28	120.88
3	C	838	OMD	C2-C1'-C6'	-2.23	118.41	120.88
3	A	838	OMD	C2-C1'-C6'	-2.08	118.58	120.88
3	A	838	OMD	C2'-C1'-C6'	2.02	120.59	118.17
3	L	838	OMD	O2-C1-C2	2.01	121.64	114.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

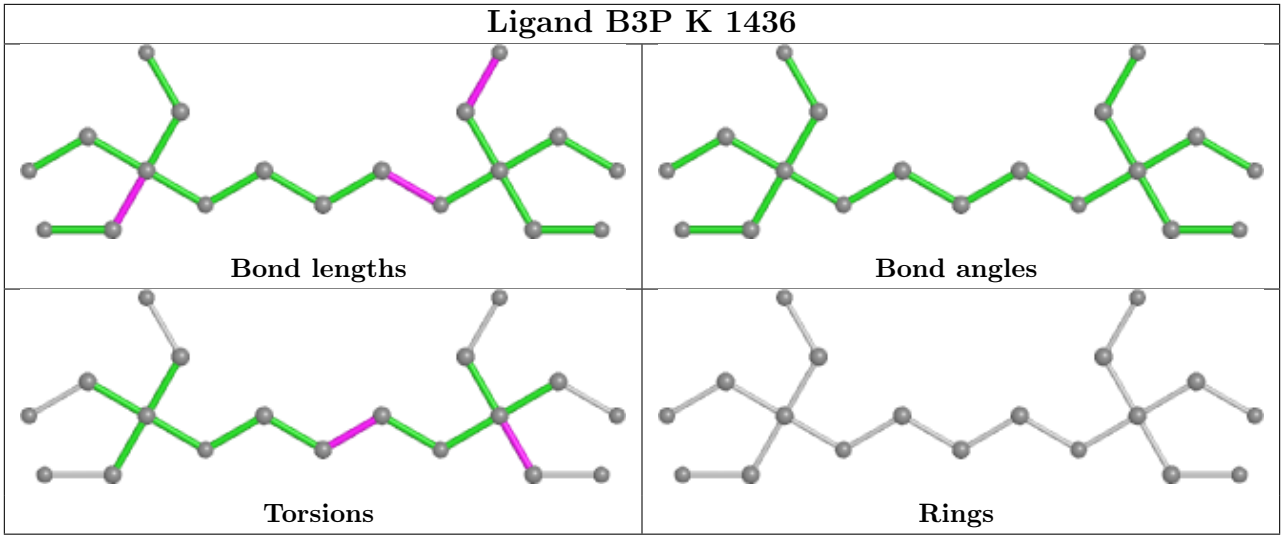
Mol	Chain	Res	Type	Atoms
4	K	1436	B3P	C3-C1-C2-N2
4	K	1436	B3P	N2-C8-C9-O1
4	K	1436	B3P	C11-C8-C9-O1
4	K	1436	B3P	C10-C8-C9-O1

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1436	B3P	1	0
3	H	838	OMD	1	0
3	D	838	OMD	1	0
3	C	838	OMD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	425/433 (98%)	-0.47	2 (0%)	91	91	9, 16, 30, 41	0
1	B	425/433 (98%)	-0.44	3 (0%)	87	88	11, 18, 31, 52	0
1	C	425/433 (98%)	-0.44	1 (0%)	95	95	10, 17, 30, 52	5 (1%)
1	D	427/433 (98%)	-0.45	0	100	100	10, 17, 29, 48	0
1	E	426/433 (98%)	-0.43	2 (0%)	91	91	11, 17, 31, 51	1 (0%)
1	F	425/433 (98%)	-0.41	0	100	100	10, 18, 30, 57	0
1	G	425/433 (98%)	-0.16	5 (1%)	79	80	15, 24, 38, 63	2 (0%)
1	H	425/433 (98%)	-0.24	3 (0%)	87	88	14, 22, 37, 53	0
1	I	426/433 (98%)	-0.22	7 (1%)	72	73	14, 23, 37, 56	0
1	J	425/433 (98%)	-0.30	4 (0%)	84	85	14, 23, 38, 60	0
1	K	426/433 (98%)	-0.35	4 (0%)	84	85	11, 19, 33, 55	0
1	L	425/433 (98%)	-0.34	3 (0%)	87	88	13, 20, 35, 53	0
All	All	5105/5196 (98%)	-0.35	34 (0%)	87	88	9, 19, 35, 63	8 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	105	ALA	5.0
1	K	86	GLY	4.2
1	H	379	ALA	4.0
1	G	235	ALA	4.0
1	K	235	ALA	3.8
1	K	87	PRO	3.5
1	G	104	PRO	3.0
1	J	381	ASP	3.0
1	L	351	GLU	2.9
1	G	87	PRO	2.8
1	J	351	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	379	ALA	2.7
1	I	381	ASP	2.6
1	J	379	ALA	2.6
1	I	236	GLU	2.6
1	I	347	ASP	2.6
1	B	235	ALA	2.5
1	B	236	GLU	2.4
1	I	375	GLU	2.4
1	A	381[A]	ASP	2.3
1	H	88	LEU	2.3
1	J	236	GLU	2.3
1	E	8	ASP	2.3
1	I	379	ALA	2.3
1	E	379	ALA	2.2
1	H	237	GLY	2.2
1	B	237	GLY	2.2
1	A	87	PRO	2.1
1	C	237	GLY	2.1
1	I	383	ALA	2.1
1	K	379	ALA	2.1
1	I	351	GLU	2.0
1	G	416	ASP	2.0
1	L	323	ASN	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.

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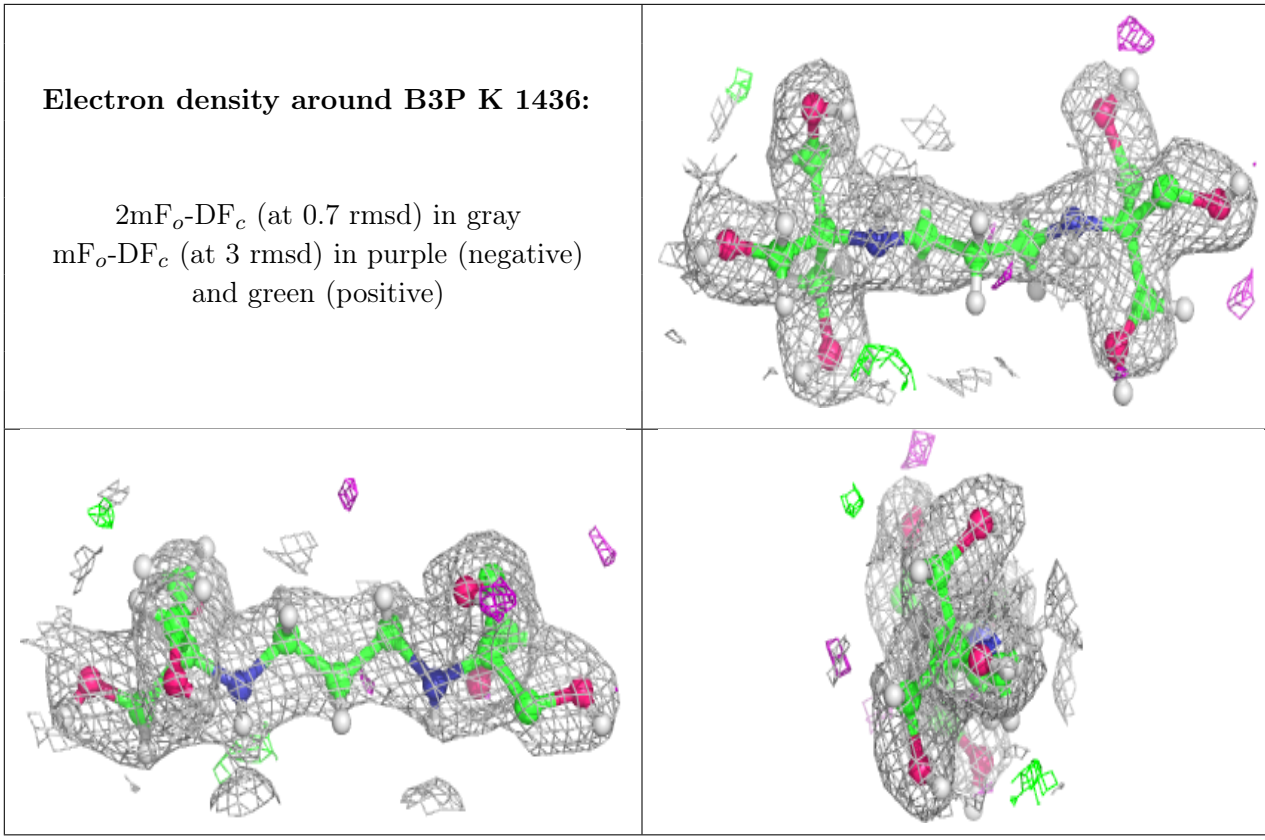
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	B3P	K	1436	19/19	0.94	0.14	18,26,33,39	0
3	OMD	L	838	12/12	0.95	0.13	18,23,24,30	0
3	OMD	D	838	12/12	0.96	0.14	12,17,19,22	0
3	OMD	F	838	12/12	0.96	0.12	13,17,18,20	0
3	OMD	G	838	12/12	0.96	0.13	17,19,23,24	0
3	OMD	J	838	12/12	0.96	0.15	18,23,25,26	12
3	OMD	A	838	12/12	0.96	0.12	8,12,15,16	0
3	OMD	C	838	12/12	0.96	0.12	9,14,16,17	12
3	OMD	H	838	12/12	0.97	0.12	18,21,24,26	0
3	OMD	E	838	12/12	0.97	0.09	11,13,15,18	0
3	OMD	K	838	12/12	0.98	0.12	15,17,20,20	0
3	OMD	I	838	12/12	0.98	0.11	20,24,26,28	0
3	OMD	B	838	12/12	0.98	0.10	13,16,18,18	0
2	FE	F	837	1/1	0.99	0.09	13,13,13,13	0
2	FE	D	837	1/1	1.00	0.07	11,11,11,11	0
2	FE	E	837	1/1	1.00	0.06	13,13,13,13	0
2	FE	A	837	1/1	1.00	0.08	11,11,11,11	0
2	FE	G	837	1/1	1.00	0.07	16,16,16,16	0
2	FE	H	837	1/1	1.00	0.07	17,17,17,17	0
2	FE	I	837	1/1	1.00	0.07	18,18,18,18	0
2	FE	J	837	1/1	1.00	0.06	16,16,16,16	0
2	FE	K	837	1/1	1.00	0.08	15,15,15,15	0
2	FE	L	837	1/1	1.00	0.07	14,14,14,14	0
2	FE	B	837	1/1	1.00	0.07	12,12,12,12	0
2	FE	C	837	1/1	1.00	0.08	11,11,11,11	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around B3P K 1436:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.