Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 09:59 pm GMT

PDB ID	:	4AQ2
Title	:	resting state of homogentisate 1,2-dioxygenase
Authors	:	Jeoung, J.-H.; Lin, T.-Y.; Bommer, M.; Dobbek, H.
Deposited on	:	2012-04-12
Resolution	:	1.95 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:

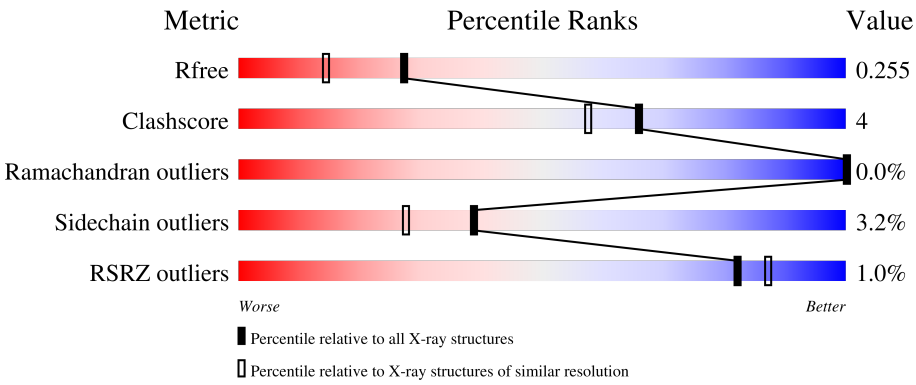
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	% 86% 12% • •
1	B	433	% 87% 11% •
1	C	433	% 88% 9% •
1	D	433	% 88% 8% • •
1	E	433	% 86% 10% • •

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

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 45534 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 HOMOGENTISATE 1,2-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	425	3346	2136	587	605	18	0	3	0
1	B	426	3353	2140	586	609	18	0	4	0
1	C	420	3308	2111	583	597	17	0	4	0
1	D	421	3306	2111	579	598	18	0	3	0
1	E	419	3286	2098	576	594	18	0	2	0
1	F	419	3304	2112	579	595	18	0	7	0
1	G	419	3307	2108	583	599	17	0	5	0
1	H	421	3345	2134	590	603	18	0	7	0
1	I	420	3296	2105	580	593	18	0	2	0
1	J	420	3297	2104	580	595	18	0	3	0
1	K	426	3338	2130	586	605	17	0	1	0
1	L	419	3289	2100	579	593	17	0	2	0

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

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

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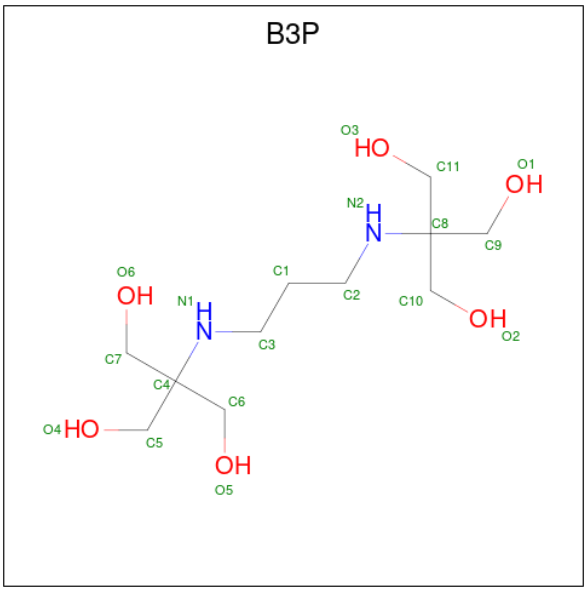
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0
2	G	1	1	1	0	0
2	H	1	1	1	0	0
2	I	1	1	1	0	0
2	J	1	1	1	0	0
2	K	1	1	1	0	0
2	L	1	1	1	0	0

- Molecule 3 is 2-[3-(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	N	O		
3	K	1	19	11	2	6	0	0

- Molecule 4 is water.

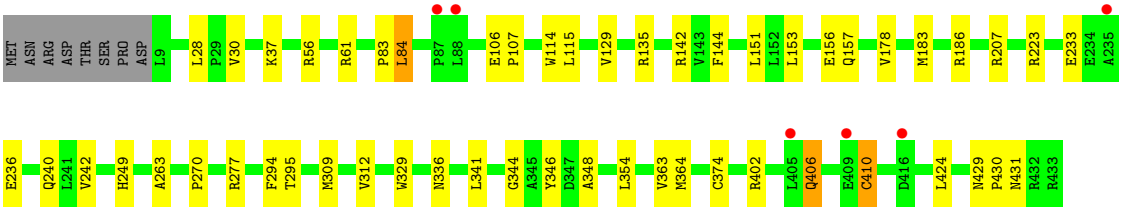
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	509	515	515	0	6
4	B	500	505	505	0	5
4	C	467	472	472	0	5
4	D	473	476	476	0	3
4	E	479	483	483	0	4
4	F	423	427	427	0	4
4	G	464	467	467	0	3
4	H	513	525	525	0	12
4	I	430	430	430	0	0
4	J	454	458	458	0	4
4	K	437	441	441	0	4
4	L	527	529	529	0	2

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.

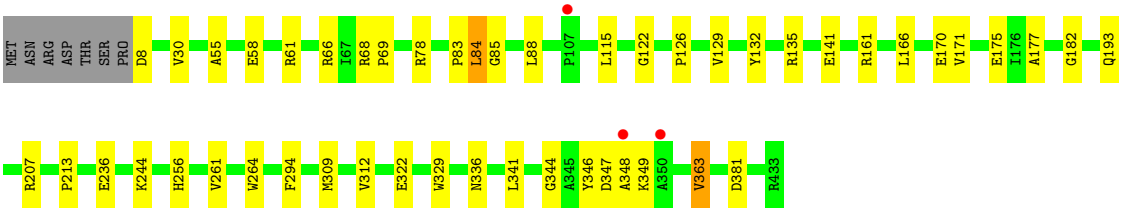
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain A:



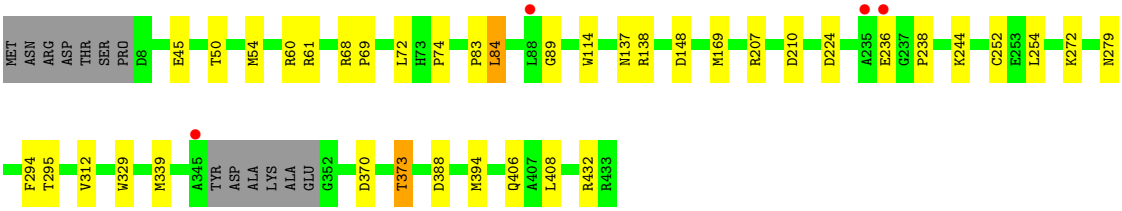
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain B:



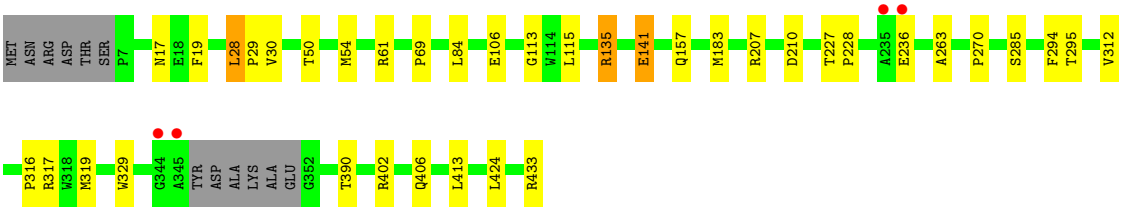
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain C:



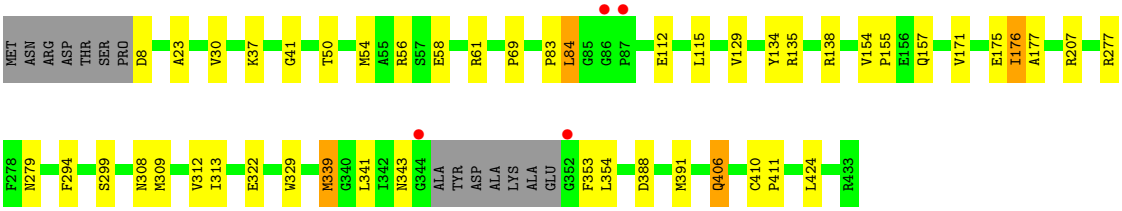
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain D:



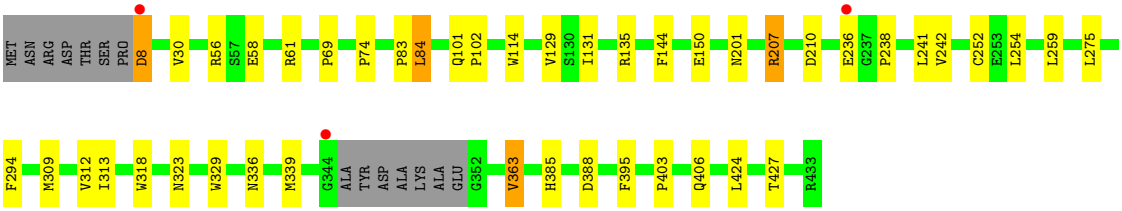
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain E:



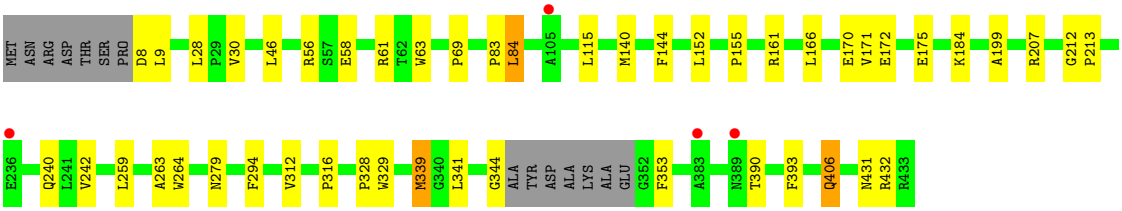
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain F:



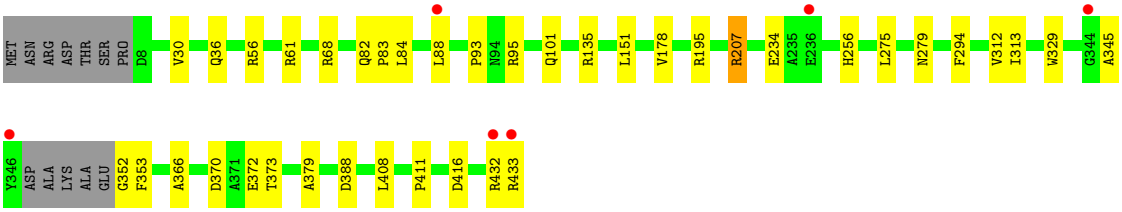
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain G:



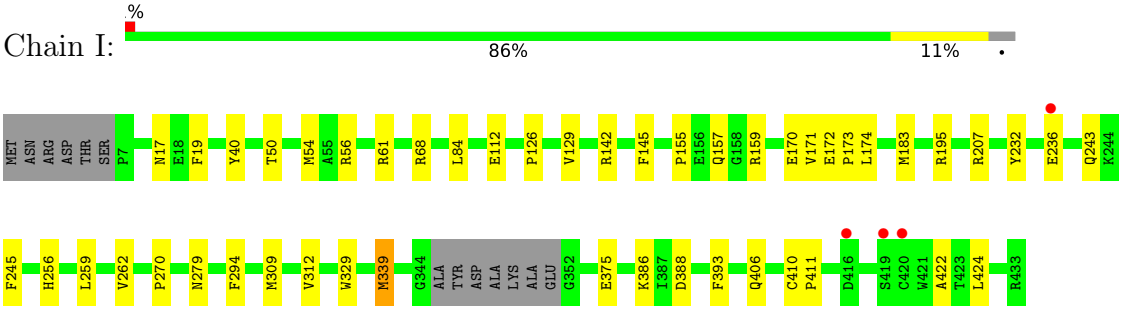
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain H:



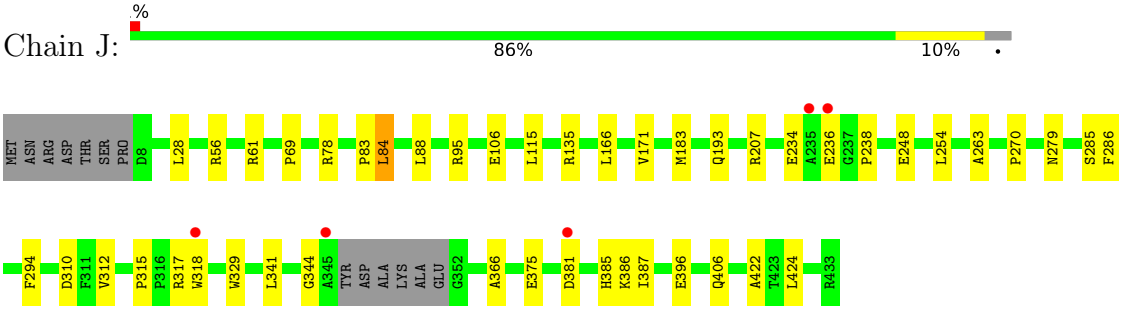
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain I:



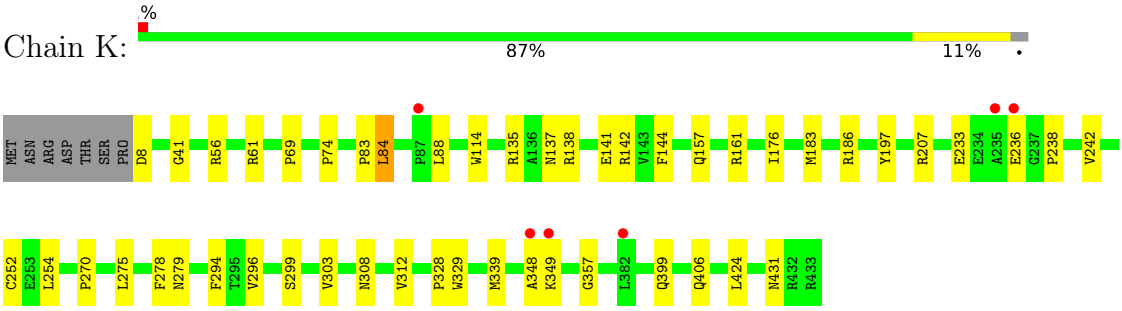
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

Chain J:



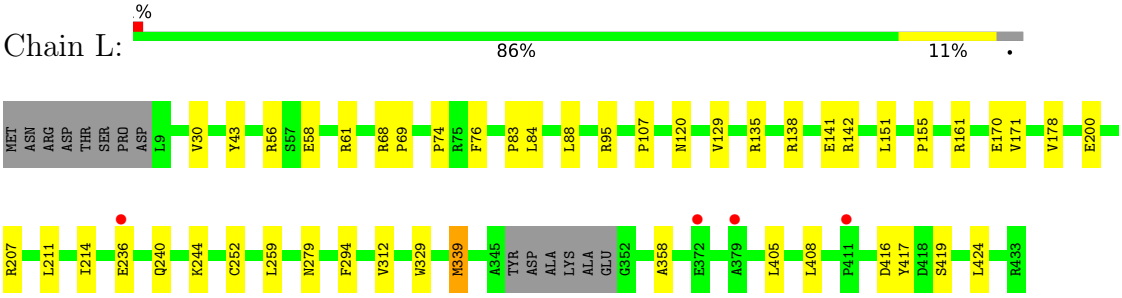
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

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	93.74Å 93.90Å 162.81Å 87.46° 80.45° 68.33°	Depositor
Resolution (Å)	33.94 – 1.95 34.31 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.8 (33.94-1.95) 94.8 (34.31-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 1.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.193 , 0.257 0.191 , 0.255	Depositor DCC
R_{free} test set	17581 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	16.3	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 66.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	45534	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% 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, 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	0.37	0/3448	0.55	0/4701
1	B	0.36	0/3458	0.55	0/4715
1	C	0.36	0/3411	0.56	0/4647
1	D	0.37	0/3407	0.56	0/4644
1	E	0.37	0/3385	0.56	0/4613
1	F	0.36	0/3409	0.56	0/4646
1	G	0.34	0/3407	0.53	0/4644
1	H	0.35	0/3446	0.55	0/4696
1	I	0.36	0/3396	0.56	0/4627
1	J	0.34	0/3396	0.55	0/4627
1	K	0.36	0/3440	0.56	0/4689
1	L	0.36	0/3389	0.54	0/4619
All	All	0.36	0/40992	0.55	0/55868

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	3346	0	3244	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3353	0	3244	28	0
1	C	3308	0	3216	24	0
1	D	3306	0	3202	22	0
1	E	3286	0	3177	29	0
1	F	3304	0	3198	33	0
1	G	3307	0	3195	26	0
1	H	3345	0	3234	28	0
1	I	3296	0	3194	26	0
1	J	3297	0	3192	24	0
1	K	3338	0	3234	30	0
1	L	3289	0	3193	25	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	K	19	0	26	3	0
4	A	515	0	0	11	0
4	B	505	0	0	10	0
4	C	472	0	0	13	0
4	D	476	0	0	9	0
4	E	483	0	0	13	0
4	F	427	0	0	9	1
4	G	467	0	0	11	1
4	H	525	0	0	19	1
4	I	430	0	0	9	1
4	J	458	0	0	11	0
4	K	441	0	0	11	0
4	L	529	0	0	7	0
All	All	45534	0	38549	314	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 4.

All (314) 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:F:56:ARG:CD	1:F:56:ARG:CB	2.49	0.90
1:H:56:ARG:CB	1:H:56:ARG:CD	2.51	0.89
1:E:56:ARG:CB	1:E:56:ARG:CD	2.50	0.89
1:J:56:ARG:CB	1:J:56:ARG:CD	2.51	0.89
1:I:56:ARG:CD	1:I:56:ARG:CB	2.52	0.86
1:A:294:PHE:HB2	1:A:312:VAL:HG13	1.65	0.78
1:K:69:PRO:HG2	1:L:424:LEU:HD13	1.67	0.76
1:A:223:ARG:NH2	4:A:2350:HOH:O	2.18	0.76
1:C:169:MET:SD	4:C:2264:HOH:O	2.45	0.74
1:D:319:MET:SD	4:D:2381:HOH:O	2.44	0.74
1:D:402:ARG:NH2	4:D:2158:HOH:O	2.21	0.72
1:K:197:TYR:OH	4:K:2273:HOH:O	2.07	0.72
1:G:294:PHE:HB2	1:G:312:VAL:HG13	1.71	0.71
1:B:135:ARG:NH2	4:B:2209:HOH:O	2.23	0.71
1:G:184:LYS:NZ	4:G:2278:HOH:O	2.20	0.71
1:A:157:GLN:NE2	4:A:2282:HOH:O	2.23	0.70
1:K:161:ARG:NH1	4:K:2252:HOH:O	2.22	0.69
4:C:2306:HOH:O	1:F:56:ARG:NH1	2.26	0.69
1:J:106:GLU:OE1	4:J:2178:HOH:O	2.09	0.69
1:H:411:PRO:O	4:H:2496:HOH:O	2.10	0.69
1:J:385:HIS:ND1	4:J:2412:HOH:O	2.24	0.68
1:E:58:GLU:OE1	4:E:2124:HOH:O	2.12	0.68
1:C:224:ASP:N	4:C:2314:HOH:O	2.28	0.67
1:D:141:GLU:O	4:D:2245:HOH:O	2.12	0.67
1:K:41:GLY:O	4:K:2069:HOH:O	2.13	0.67
1:E:322:GLU:OE2	4:E:2394:HOH:O	2.13	0.66
1:B:55:ALA:HB3	1:B:58[A]:GLU:HG3	1.78	0.65
1:E:83:PRO:HB2	1:E:84:LEU:HD13	1.78	0.65
1:B:132:TYR:OH	4:B:2240:HOH:O	2.13	0.65
1:C:294:PHE:HB2	1:C:312:VAL:HG13	1.79	0.65
1:I:386:LYS:O	4:I:2399:HOH:O	2.15	0.65
1:D:157:GLN:NE2	4:D:2273:HOH:O	2.31	0.64
1:K:294:PHE:HB2	1:K:312:VAL:HG13	1.79	0.64
1:I:157:GLN:OE1	4:I:2242:HOH:O	2.14	0.64
1:G:58:GLU:OE2	4:G:2121:HOH:O	2.14	0.64
1:K:84:LEU:HD11	1:K:114:TRP:HB2	1.80	0.64
1:D:28:LEU:HD13	1:D:263:ALA:HB1	1.80	0.63
1:B:161:ARG:NH1	1:B:170:GLU:OE2	2.31	0.63
1:A:151:LEU:O	4:A:2277:HOH:O	2.15	0.63
1:A:183:MET:SD	4:A:2290:HOH:O	2.56	0.63
1:G:432[A]:ARG:NH1	4:G:2463:HOH:O	2.31	0.63
1:B:83:PRO:HB2	1:B:84:LEU:HD13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432[B]:ARG:NH2	4:C:2465:HOH:O	2.23	0.62
1:I:375:GLU:OE1	4:I:2390:HOH:O	2.16	0.62
1:L:161:ARG:NH1	1:L:170:GLU:OE2	2.33	0.62
1:C:83:PRO:HB2	1:C:84:LEU:HD13	1.82	0.61
1:D:294:PHE:HB2	1:D:312:VAL:HG13	1.83	0.61
1:H:416:ASP:OD1	4:H:2503:HOH:O	2.16	0.61
1:H:433:ARG:NH1	4:H:2524:HOH:O	2.33	0.61
1:K:74:PRO:HG2	1:K:252:CYS:HB2	1.82	0.61
1:E:23:ALA:O	4:E:2053:HOH:O	2.16	0.60
1:K:157:GLN:NE2	4:K:2244:HOH:O	2.32	0.60
1:L:74:PRO:HG2	1:L:252:CYS:HB2	1.83	0.60
1:J:317:ARG:NH2	4:J:2367:HOH:O	2.33	0.60
1:J:310:ASP:OD2	4:J:2363:HOH:O	2.16	0.59
1:F:83:PRO:HB2	1:F:84:LEU:HD13	1.84	0.59
1:K:142:ARG:HD3	3:K:1434:B3P:H51	1.85	0.59
1:L:294:PHE:HB2	1:L:312:VAL:HG13	1.85	0.59
1:H:207:ARG:NH1	4:H:2313:HOH:O	2.32	0.59
1:G:83:PRO:HB2	1:G:84:LEU:HD13	1.85	0.58
1:I:294:PHE:HB2	1:I:312:VAL:HG13	1.86	0.57
1:D:424:LEU:HD13	1:F:69:PRO:HG2	1.87	0.57
1:J:375:GLU:OE2	4:J:2406:HOH:O	2.17	0.57
1:K:431:ASN:O	4:K:2434:HOH:O	2.17	0.57
1:H:432[A]:ARG:NH1	4:H:2521:HOH:O	2.38	0.57
1:E:294:PHE:HB2	1:E:312:VAL:HG13	1.85	0.57
1:K:176:ILE:N	4:K:2259:HOH:O	2.38	0.56
1:L:200:GLU:OE2	1:L:244:LYS:NZ	2.34	0.56
1:C:272:LYS:HB3	4:C:2264:HOH:O	2.04	0.56
1:H:101:GLN:O	1:H:195:ARG:NH1	2.35	0.56
1:A:430:PRO:HB3	4:B:2347:HOH:O	2.06	0.56
1:J:193:GLN:O	4:J:2252[A]:HOH:O	2.17	0.56
1:J:28:LEU:HD13	1:J:263:ALA:HB1	1.86	0.56
1:B:88:LEU:HD11	1:B:122:GLY:HA2	1.88	0.56
1:D:295:THR:HG23	4:D:2363:HOH:O	2.06	0.56
1:H:408:LEU:O	4:H:2492:HOH:O	2.18	0.55
1:A:295:THR:HA	1:A:312:VAL:HG22	1.89	0.55
1:K:399:GLN:OE1	4:K:2411:HOH:O	2.18	0.55
1:B:348:ALA:HB3	1:B:349:LYS:HE3	1.88	0.55
1:G:56:ARG:NH2	4:G:2100:HOH:O	2.33	0.55
1:G:432[B]:ARG:NH2	4:G:2466:HOH:O	2.38	0.55
4:C:2292:HOH:O	1:F:56:ARG:NH2	2.11	0.55
1:H:370:ASP:HB3	4:H:2456:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:LEU:HD13	1:G:263:ALA:HB1	1.87	0.55
1:B:193:GLN:OE1	4:B:2303:HOH:O	2.18	0.54
1:E:69:PRO:HG2	1:F:424:LEU:HD13	1.89	0.54
1:E:138:ARG:NE	4:E:2243:HOH:O	2.26	0.54
4:J:2166:HOH:O	1:L:76:PHE:O	2.18	0.54
1:A:56:ARG:NH2	4:A:2112:HOH:O	2.21	0.54
1:A:153:LEU:HG	4:A:2277:HOH:O	2.07	0.54
1:K:186:ARG:NH2	1:K:233:GLU:OE2	2.26	0.54
1:I:183:MET:SD	1:I:270:PRO:HD3	2.47	0.54
1:L:405:LEU:O	4:L:2376:HOH:O	2.18	0.54
1:A:186:ARG:NH2	1:A:233:GLU:OE2	2.26	0.54
1:L:68:ARG:NH1	4:L:2094:HOH:O	2.40	0.54
4:C:2295:HOH:O	1:D:210:ASP:OD2	2.18	0.54
1:C:89:GLY:HA3	1:C:408:LEU:HD12	1.89	0.53
1:L:138:ARG:NH1	4:L:2194:HOH:O	2.41	0.53
1:C:74:PRO:HG2	1:C:252:CYS:HB2	1.89	0.53
1:A:142:ARG:HD3	1:A:240:GLN:OE1	2.09	0.53
1:B:347:ASP:HB3	4:B:2406:HOH:O	2.08	0.53
1:K:357:GLY:N	4:K:2273:HOH:O	2.41	0.53
1:D:317:ARG:HG3	4:D:2381:HOH:O	2.08	0.53
4:G:2386:HOH:O	1:H:36:GLN:OE1	2.18	0.53
1:H:352:GLY:N	4:H:2442:HOH:O	2.42	0.52
1:B:129:VAL:HG21	1:B:309:MET:HB3	1.91	0.52
1:E:277:ARG:NH1	4:E:2325:HOH:O	2.42	0.52
1:H:379:ALA:O	4:H:2466:HOH:O	2.19	0.52
1:K:83:PRO:HB2	1:K:84:LEU:HD13	1.91	0.52
1:H:83:PRO:HD2	4:H:2155:HOH:O	2.10	0.51
1:I:126:PRO:O	4:I:2204:HOH:O	2.19	0.51
1:I:129:VAL:HG21	1:I:309:MET:HB3	1.91	0.51
1:A:84:LEU:HD11	1:A:114:TRP:HB2	1.93	0.51
1:E:112:GLU:O	4:E:2155:HOH:O	2.19	0.51
1:F:135:ARG:NH2	4:F:2176:HOH:O	2.43	0.51
1:L:58:GLU:OE1	4:L:2083:HOH:O	2.19	0.51
1:F:114:TRP:HH2	4:F:2234:HOH:O	1.93	0.51
1:G:339:MET:HE3	1:G:393:PHE:O	2.10	0.51
1:J:424:LEU:HD13	1:L:69:PRO:HG2	1.91	0.51
1:F:74:PRO:HG2	1:F:252:CYS:HB2	1.93	0.51
1:C:148:ASP:OD2	1:C:244:LYS:NZ	2.40	0.51
1:J:294:PHE:HB2	1:J:312:VAL:HG13	1.93	0.51
1:H:56:ARG:NH2	4:H:2110:HOH:O	2.37	0.50
1:B:294:PHE:HB2	1:B:312:VAL:HG13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:MET:SD	1:D:270:PRO:HD3	2.52	0.50
1:G:46:LEU:HD13	1:G:63:TRP:CE2	2.46	0.50
1:A:129:VAL:HG21	1:A:309:MET:HB3	1.93	0.50
1:D:50:THR:HB	1:D:54:MET:HG3	1.92	0.50
1:K:275:LEU:HG	4:K:2259:HOH:O	2.11	0.50
1:C:84:LEU:HD11	1:C:114:TRP:HB2	1.93	0.49
1:L:95:ARG:HB2	4:L:2141:HOH:O	2.11	0.49
1:K:349:LYS:HE2	4:K:2380:HOH:O	2.11	0.49
1:B:322:GLU:OE2	1:F:318:TRP:NE1	2.44	0.49
1:B:349:LYS:NZ	4:B:2447:HOH:O	2.42	0.49
1:F:241:LEU:HD22	1:F:254:LEU:HD11	1.94	0.49
1:G:9:LEU:HD12	1:G:170:GLU:HG3	1.94	0.49
1:D:413:LEU:O	4:D:2453:HOH:O	2.20	0.49
1:J:396:GLU:OE1	4:J:2419:HOH:O	2.20	0.49
1:E:157:GLN:OE1	4:E:2267:HOH:O	2.19	0.48
4:E:2063:HOH:O	1:F:323:ASN:HB3	2.13	0.48
1:F:339:MET:HG3	4:F:2369:HOH:O	2.12	0.48
1:I:422:ALA:O	4:I:2420:HOH:O	2.20	0.48
1:C:50:THR:HB	1:C:54:MET:HG3	1.96	0.48
1:C:370:ASP:OD1	1:C:373[A]:THR:OG1	2.27	0.48
1:J:83:PRO:HB2	1:J:84:LEU:HD13	1.95	0.48
1:G:406:GLN:H	1:G:406:GLN:CD	2.17	0.48
1:C:45:GLU:HG2	4:C:2075:HOH:O	2.13	0.48
1:F:101:GLN:NE2	4:F:2162:HOH:O	2.46	0.48
1:J:422:ALA:O	4:J:2442:HOH:O	2.20	0.48
1:E:8:ASP:HB3	4:E:2013:HOH:O	2.13	0.47
1:B:336:ASN:OD1	1:B:363[B]:VAL:HG13	2.15	0.47
1:E:37:LYS:HA	4:E:2072:HOH:O	2.14	0.47
1:J:234:GLU:OE2	4:J:2315:HOH:O	2.20	0.47
1:F:8:ASP:OD1	1:F:8:ASP:N	2.48	0.47
1:B:126:PRO:HA	4:B:2219:HOH:O	2.14	0.47
1:C:295:THR:HA	1:C:312:VAL:HG22	1.95	0.47
1:C:339:MET:HG2	1:C:394:MET:HB2	1.97	0.47
1:E:50:THR:HB	1:E:54:MET:HG3	1.95	0.47
1:E:406:GLN:H	1:E:406:GLN:CD	2.18	0.47
1:F:8:ASP:HB3	4:F:2004:HOH:O	2.15	0.47
1:G:69:PRO:HG2	1:I:424:LEU:HD13	1.97	0.47
1:A:429:ASN:HA	1:A:430:PRO:HD2	1.78	0.47
1:E:171:VAL:HG21	1:E:177:ALA:HB2	1.96	0.47
1:F:336:ASN:OD1	1:F:363[B]:VAL:HG23	2.14	0.47
1:E:138:ARG:NH2	4:E:2244:HOH:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:120:ASN:OD1	1:L:129:VAL:N	2.41	0.46
1:F:294:PHE:HB2	1:F:312:VAL:HG13	1.98	0.46
1:J:69:PRO:HG2	1:K:424:LEU:HD13	1.96	0.46
1:H:433:ARG:HB2	1:I:40:TYR:CZ	2.50	0.46
1:I:50:THR:HB	1:I:54:MET:HG3	1.97	0.46
1:K:183:MET:SD	1:K:270:PRO:HD3	2.55	0.46
1:F:102:PRO:O	4:F:2163:HOH:O	2.21	0.46
1:L:408:LEU:HB2	4:L:2376:HOH:O	2.15	0.46
1:A:277:ARG:NE	4:A:2382:HOH:O	2.49	0.46
1:C:68:ARG:HD3	1:C:72:LEU:HD23	1.96	0.46
4:J:2352:HOH:O	1:K:303:VAL:HG22	2.14	0.46
1:D:433:ARG:NH2	4:D:2469:HOH:O	2.48	0.46
1:K:299:SER:O	1:K:308:ASN:N	2.49	0.46
1:B:346:TYR:HD2	1:B:349:LYS:HG2	1.81	0.45
1:G:175:GLU:OE2	4:G:2269:HOH:O	2.20	0.45
1:L:107:PRO:HG3	1:L:138:ARG:NH2	2.31	0.45
4:I:2282:HOH:O	1:L:56:ARG:NH2	2.37	0.45
4:C:2182:HOH:O	1:D:285:SER:HB2	2.16	0.45
1:F:84:LEU:HD11	1:F:114:TRP:HB2	1.98	0.45
1:G:152:LEU:HB3	1:G:199:ALA:HB3	1.99	0.45
1:K:141:GLU:OE1	3:K:1434:B3P:N2	2.49	0.45
1:A:156:GLU:OE2	1:A:157:GLN:HG3	2.17	0.45
1:G:144:PHE:HA	1:G:242:VAL:O	2.16	0.45
1:L:83:PRO:HG2	1:L:84:LEU:HD13	1.98	0.45
1:B:166:LEU:HD13	1:B:264:TRP:CD2	2.52	0.45
1:B:341:LEU:HD21	1:B:344:GLY:O	2.16	0.45
1:C:238:PRO:HA	1:C:254:LEU:O	2.16	0.45
1:G:140:MET:HG3	4:G:2196:HOH:O	2.16	0.45
1:H:93:PRO:HB3	1:I:245:PHE:CG	2.51	0.45
1:H:151:LEU:O	1:H:178:VAL:HA	2.17	0.45
1:I:68:ARG:HD2	1:I:256:HIS:CG	2.52	0.45
1:J:238:PRO:HA	1:J:254:LEU:O	2.17	0.45
1:K:137:ASN:OD1	1:K:138:ARG:HG2	2.17	0.44
1:L:142:ARG:HD3	1:L:240:GLN:OE1	2.17	0.44
1:I:339:MET:HE3	1:I:393:PHE:O	2.17	0.44
1:H:275:LEU:HD22	1:H:313:ILE:HG21	1.99	0.44
1:I:195:ARG:NH2	4:I:2242:HOH:O	2.51	0.44
1:L:43:TYR:CD2	1:L:69:PRO:HD3	2.53	0.44
1:A:402:ARG:NH1	4:A:2485:HOH:O	2.50	0.44
1:A:144:PHE:HA	1:A:242:VAL:O	2.17	0.44
1:D:17:ASN:HB2	1:D:19:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:GLU:HG3	4:D:2189:HOH:O	2.17	0.44
1:G:328:PRO:HD3	4:G:2357:HOH:O	2.16	0.44
1:L:151:LEU:O	1:L:178:VAL:HA	2.17	0.44
1:E:134:TYR:HB2	4:E:2204:HOH:O	2.17	0.44
1:I:112:GLU:OE2	1:I:142:ARG:NH2	2.51	0.44
1:J:95:ARG:HD3	1:J:366:ALA:O	2.17	0.44
1:L:339:MET:O	1:L:358:ALA:HA	2.18	0.44
1:C:83:PRO:HG3	4:C:2132:HOH:O	2.18	0.43
1:J:318:TRP:NE1	1:J:386:LYS:HD3	2.33	0.43
1:A:28:LEU:HG	1:A:263:ALA:HB1	1.99	0.43
1:J:166:LEU:HD12	1:J:270:PRO:HD2	2.01	0.43
1:C:68:ARG:HA	1:C:69:PRO:HD3	1.91	0.43
1:D:113:GLY:HA3	1:D:135:ARG:O	2.18	0.43
1:A:341:LEU:HD23	1:A:354:LEU:C	2.38	0.43
1:E:129:VAL:HG21	1:E:309:MET:HB3	2.00	0.43
1:G:316:PRO:HD3	1:G:390:THR:O	2.18	0.43
1:I:410:CYS:HA	1:I:411:PRO:HD3	1.82	0.43
1:E:155:PRO:HD2	1:E:175:GLU:O	2.19	0.43
1:G:240:GLN:NE2	4:G:2330:HOH:O	2.51	0.43
1:C:84:LEU:HD23	1:C:244:LYS:HE2	2.00	0.43
1:F:30:VAL:HG12	4:F:2053:HOH:O	2.17	0.43
1:F:58[B]:GLU:OE1	1:F:207:ARG:NH1	2.43	0.43
1:G:155:PRO:HD2	1:G:175:GLU:O	2.19	0.43
1:H:68:ARG:NH2	4:H:2137:HOH:O	2.51	0.43
1:H:433:ARG:HD2	4:H:2525:HOH:O	2.18	0.43
4:H:2318:HOH:O	1:K:56:ARG:NH2	2.30	0.43
1:I:17:ASN:HB2	1:I:19:PHE:CZ	2.54	0.43
1:K:328:PRO:HG2	1:K:348:ALA:HB2	2.01	0.43
1:B:84:LEU:HD23	1:B:244:LYS:HE2	2.00	0.42
1:E:294:PHE:HB3	1:E:313:ILE:O	2.19	0.42
1:F:129:VAL:HG21	1:F:309:MET:HB3	2.01	0.42
1:I:126:PRO:HA	4:I:2194:HOH:O	2.17	0.42
1:K:339:MET:HE2	1:K:339:MET:HB3	1.89	0.42
1:G:161:ARG:NH2	4:G:2260:HOH:O	2.41	0.42
1:A:106[A]:GLU:HG3	1:A:107:PRO:HD2	2.02	0.42
1:J:315:PRO:O	1:J:317:ARG:NH1	2.50	0.42
1:G:212:GLY:HA3	1:G:213:PRO:HD3	1.84	0.42
1:B:85:GLY:HA2	4:B:2165:HOH:O	2.19	0.42
1:D:227:THR:HG23	1:D:228:PRO:HD2	2.02	0.42
1:F:144:PHE:HA	1:F:242:VAL:O	2.19	0.42
1:F:238:PRO:HA	1:F:254:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:275:LEU:HD22	1:F:313:ILE:HD13	2.02	0.42
1:F:294:PHE:HB3	1:F:313:ILE:O	2.19	0.42
1:I:170:GLU:OE1	4:I:2250:HOH:O	2.22	0.42
1:I:232:TYR:CD1	1:I:262:VAL:HG22	2.55	0.42
1:K:144:PHE:HA	1:K:242:VAL:O	2.20	0.42
1:K:238:PRO:HA	1:K:254:LEU:O	2.19	0.42
1:A:37:LYS:HA	4:A:2069:HOH:O	2.19	0.42
1:E:41:GLY:O	1:F:427:THR:OG1	2.30	0.42
1:G:341:LEU:HD21	1:G:344:GLY:O	2.19	0.42
1:H:345:ALA:N	4:H:2441:HOH:O	2.53	0.42
1:I:155:PRO:HG2	1:I:171:VAL:HG12	2.01	0.42
1:A:83:PRO:HG2	1:A:249:HIS:CE1	2.54	0.42
1:A:341:LEU:HD21	1:A:344:GLY:O	2.20	0.42
1:A:346:TYR:CE2	1:A:348:ALA:HB3	2.54	0.42
1:A:431:ASN:ND2	4:A:2507:HOH:O	2.52	0.42
1:E:138:ARG:NH1	4:E:2239:HOH:O	2.52	0.42
1:F:131:ILE:HD13	1:F:395:PHE:HD2	1.85	0.42
1:A:183:MET:SD	1:A:270:PRO:HD3	2.59	0.41
1:C:406:GLN:NE2	4:C:2142:HOH:O	2.53	0.41
1:D:316:PRO:HD3	1:D:390:THR:O	2.20	0.41
1:F:403:PRO:HD2	4:F:2134:HOH:O	2.20	0.41
1:H:373[A]:THR:HG23	4:H:2454:HOH:O	2.21	0.41
1:A:336:ASN:OD1	1:A:363:VAL:HG23	2.20	0.41
4:A:2350:HOH:O	1:D:29:PRO:O	2.22	0.41
1:B:68:ARG:HD2	1:B:256:HIS:CG	2.55	0.41
1:C:137:ASN:O	1:C:138:ARG:HD3	2.21	0.41
1:G:172:GLU:O	1:G:175:GLU:HB2	2.21	0.41
1:H:234:GLU:OE1	4:H:2357:HOH:O	2.22	0.41
1:A:364:MET:HG3	1:B:182:GLY:HA3	2.02	0.41
1:B:213:PRO:HD3	1:F:210:ASP:O	2.20	0.41
1:K:278:PHE:CE1	1:K:296:VAL:HG22	2.55	0.41
3:K:1434:B3P:H52	3:K:1434:B3P:H32	1.86	0.41
1:B:78:ARG:NH2	4:B:2155:HOH:O	2.36	0.41
1:B:175:GLU:OE2	4:B:2292:HOH:O	2.21	0.41
1:F:150:GLU:HB3	1:F:201:ASN:HB3	2.03	0.41
1:H:68:ARG:HD2	1:H:256:HIS:CG	2.56	0.41
1:E:341:LEU:HD12	1:E:391:MET:O	2.21	0.41
1:I:173:PRO:O	1:I:174:LEU:HB2	2.21	0.41
1:J:285:SER:OG	1:J:286:PHE:N	2.53	0.41
1:F:385:HIS:HB2	4:F:2389:HOH:O	2.21	0.41
1:H:372:GLU:HB3	4:H:2454:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:339:MET:HG3	4:K:2368:HOH:O	2.20	0.41
1:E:410:CYS:HA	1:E:411:PRO:HD3	1.92	0.41
1:G:166:LEU:HB3	1:G:264:TRP:CE2	2.56	0.41
1:H:95:ARG:HD3	1:H:366:ALA:O	2.20	0.41
1:H:294:PHE:HB2	1:H:312:VAL:HG13	2.03	0.41
1:I:145:PHE:O	1:I:243:GLN:HA	2.20	0.41
1:J:183:MET:SD	1:J:270:PRO:HD3	2.60	0.41
1:J:341:LEU:HD21	1:J:344:GLY:O	2.20	0.41
1:L:155:PRO:HG2	1:L:171:VAL:HG12	2.02	0.41
1:L:416:ASP:O	1:L:419:SER:OG	2.37	0.41
1:B:171:VAL:HG21	1:B:177:ALA:HB2	2.03	0.41
1:D:69:PRO:HG2	1:E:424:LEU:HD13	2.01	0.41
1:E:299:SER:O	1:E:308:ASN:N	2.53	0.41
1:E:339:MET:HE2	1:E:339:MET:HB3	1.92	0.41
1:B:66:ARG:HB3	1:B:261:VAL:HG22	2.03	0.40
1:C:210:ASP:HB2	4:C:2298:HOH:O	2.20	0.40
1:L:417:TYR:HA	4:L:2144:HOH:O	2.21	0.40
1:I:159:ARG:HG2	1:I:172:GLU:CB	2.51	0.40
1:A:424:LEU:HD13	1:B:69:PRO:HG2	2.01	0.40
1:A:406:GLN:O	1:A:410:CYS:HB3	2.21	0.40
1:C:60:ARG:HD2	4:C:2104:HOH:O	2.20	0.40
1:H:82:GLN:HA	4:H:2155:HOH:O	2.20	0.40
1:A:151:LEU:O	1:A:178:VAL:HA	2.21	0.40
1:E:154:VAL:HG22	1:E:176:ILE:HG22	2.03	0.40
1:J:78:ARG:HE	1:J:248:GLU:CD	2.25	0.40
1:L:211:LEU:HB3	1:L:214:ILE:HB	2.03	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)
4:H:2293:HOH:O	4:I:2426:HOH:O[1_565]	2.10	0.10
4:F:2255:HOH:O	4:G:2189:HOH:O[1_465]	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	426/433 (98%)	416 (98%)	10 (2%)	0	100	100
1	B	428/433 (99%)	413 (96%)	13 (3%)	2 (0%)	29	17
1	C	419/433 (97%)	408 (97%)	11 (3%)	0	100	100
1	D	420/433 (97%)	409 (97%)	11 (3%)	0	100	100
1	E	417/433 (96%)	403 (97%)	14 (3%)	0	100	100
1	F	421/433 (97%)	407 (97%)	12 (3%)	2 (0%)	29	17
1	G	419/433 (97%)	408 (97%)	11 (3%)	0	100	100
1	H	424/433 (98%)	410 (97%)	14 (3%)	0	100	100
1	I	418/433 (96%)	407 (97%)	11 (3%)	0	100	100
1	J	418/433 (96%)	408 (98%)	10 (2%)	0	100	100
1	K	425/433 (98%)	414 (97%)	11 (3%)	0	100	100
1	L	417/433 (96%)	406 (97%)	11 (3%)	0	100	100
All	All	5052/5196 (97%)	4909 (97%)	139 (3%)	4 (0%)	100	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	363[A]	VAL
1	F	363[B]	VAL
1	B	363[A]	VAL
1	B	363[B]	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	349/355 (98%)	338 (97%)	11 (3%)	39	27
1	B	350/355 (99%)	340 (97%)	10 (3%)	42	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	347/355 (98%)	338 (97%)	9 (3%)	46	36
1	D	346/355 (98%)	335 (97%)	11 (3%)	39	27
1	E	343/355 (97%)	328 (96%)	15 (4%)	28	15
1	F	345/355 (97%)	336 (97%)	9 (3%)	46	36
1	G	346/355 (98%)	332 (96%)	14 (4%)	31	19
1	H	349/355 (98%)	339 (97%)	10 (3%)	42	31
1	I	344/355 (97%)	334 (97%)	10 (3%)	42	31
1	J	344/355 (97%)	331 (96%)	13 (4%)	33	21
1	K	348/355 (98%)	338 (97%)	10 (3%)	42	31
1	L	344/355 (97%)	333 (97%)	11 (3%)	39	27
All	All	4155/4260 (98%)	4022 (97%)	133 (3%)	39	27

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	61	ARG
1	A	84	LEU
1	A	115	LEU
1	A	135	ARG
1	A	207	ARG
1	A	236	GLU
1	A	329	TRP
1	A	374	CYS
1	A	406	GLN
1	A	410	CYS
1	B	8	ASP
1	B	30	VAL
1	B	61	ARG
1	B	84	LEU
1	B	115	LEU
1	B	141	GLU
1	B	207	ARG
1	B	236	GLU
1	B	329	TRP
1	B	381	ASP
1	C	61	ARG
1	C	84	LEU

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Mol	Chain	Res	Type
1	C	207	ARG
1	C	236	GLU
1	C	279	ASN
1	C	329	TRP
1	C	373[A]	THR
1	C	373[B]	THR
1	C	388	ASP
1	D	28	LEU
1	D	30	VAL
1	D	61	ARG
1	D	84	LEU
1	D	115	LEU
1	D	135	ARG
1	D	141	GLU
1	D	207	ARG
1	D	236	GLU
1	D	329	TRP
1	D	406	GLN
1	E	30	VAL
1	E	61	ARG
1	E	84	LEU
1	E	115	LEU
1	E	135	ARG
1	E	176	ILE
1	E	207	ARG
1	E	279	ASN
1	E	329	TRP
1	E	339	MET
1	E	343	ASN
1	E	353	PHE
1	E	354	LEU
1	E	388	ASP
1	E	406	GLN
1	F	8	ASP
1	F	61	ARG
1	F	84	LEU
1	F	207	ARG
1	F	236	GLU
1	F	259	LEU
1	F	329	TRP
1	F	388	ASP
1	F	406	GLN

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Mol	Chain	Res	Type
1	G	8	ASP
1	G	30	VAL
1	G	61	ARG
1	G	84	LEU
1	G	115	LEU
1	G	171	VAL
1	G	207	ARG
1	G	259	LEU
1	G	279	ASN
1	G	329	TRP
1	G	339	MET
1	G	353	PHE
1	G	406	GLN
1	G	431	ASN
1	H	30	VAL
1	H	61	ARG
1	H	84	LEU
1	H	88	LEU
1	H	135	ARG
1	H	207	ARG
1	H	279	ASN
1	H	329	TRP
1	H	353	PHE
1	H	388	ASP
1	I	61	ARG
1	I	84	LEU
1	I	207	ARG
1	I	236	GLU
1	I	259	LEU
1	I	279	ASN
1	I	329	TRP
1	I	339	MET
1	I	388	ASP
1	I	406	GLN
1	J	61	ARG
1	J	84	LEU
1	J	88	LEU
1	J	115	LEU
1	J	135	ARG
1	J	171	VAL
1	J	207	ARG
1	J	236	GLU

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Mol	Chain	Res	Type
1	J	279	ASN
1	J	329	TRP
1	J	381	ASP
1	J	387	ILE
1	J	406	GLN
1	K	8	ASP
1	K	61	ARG
1	K	84	LEU
1	K	88	LEU
1	K	135	ARG
1	K	207	ARG
1	K	236	GLU
1	K	279	ASN
1	K	329	TRP
1	K	406	GLN
1	L	30	VAL
1	L	61	ARG
1	L	88	LEU
1	L	135	ARG
1	L	141	GLU
1	L	207	ARG
1	L	236	GLU
1	L	259	LEU
1	L	279	ASN
1	L	329	TRP
1	L	339	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	B	157	GLN
1	B	231	HIS
1	B	243	GLN
1	C	243	GLN
1	D	193	GLN
1	D	389	ASN
1	E	157	GLN
1	E	385	HIS
1	F	231	HIS
1	G	157	GLN
1	G	343	ASN

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Mol	Chain	Res	Type
1	H	36	GLN
1	I	157	GLN
1	J	193	GLN
1	K	304	HIS
1	K	399	GLN
1	L	157	GLN
1	L	193	GLN
1	L	431	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 13 ligands modelled in this entry, 12 are monoatomic - leaving 1 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	B3P	K	1434	-	18,18,18	1.53	3 (16%)	21,23,23	1.80	8 (38%)

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	B3P	K	1434	-	-	6/28/28/28	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1434	B3P	C5-C4	-3.65	1.49	1.53
3	K	1434	B3P	C6-C4	-2.26	1.50	1.53
3	K	1434	B3P	C11-C8	-2.02	1.51	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	1434	B3P	C2-N2-C8	-3.38	111.28	116.08
3	K	1434	B3P	O3-C11-C8	3.26	118.23	111.63
3	K	1434	B3P	O6-C7-C4	2.95	117.61	111.63
3	K	1434	B3P	O1-C9-C8	2.91	117.53	111.63
3	K	1434	B3P	O2-C10-C8	2.70	117.11	111.63
3	K	1434	B3P	O5-C6-C4	2.28	116.24	111.63
3	K	1434	B3P	C3-N1-C4	-2.14	113.03	116.08
3	K	1434	B3P	O4-C5-C4	2.01	115.70	111.63

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	1434	B3P	C6-C4-C5-O4
3	K	1434	B3P	C7-C4-C5-O4
3	K	1434	B3P	O3-C11-C8-N2
3	K	1434	B3P	O3-C11-C8-C9
3	K	1434	B3P	O3-C11-C8-C10
3	K	1434	B3P	N1-C4-C5-O4

There are no ring outliers.

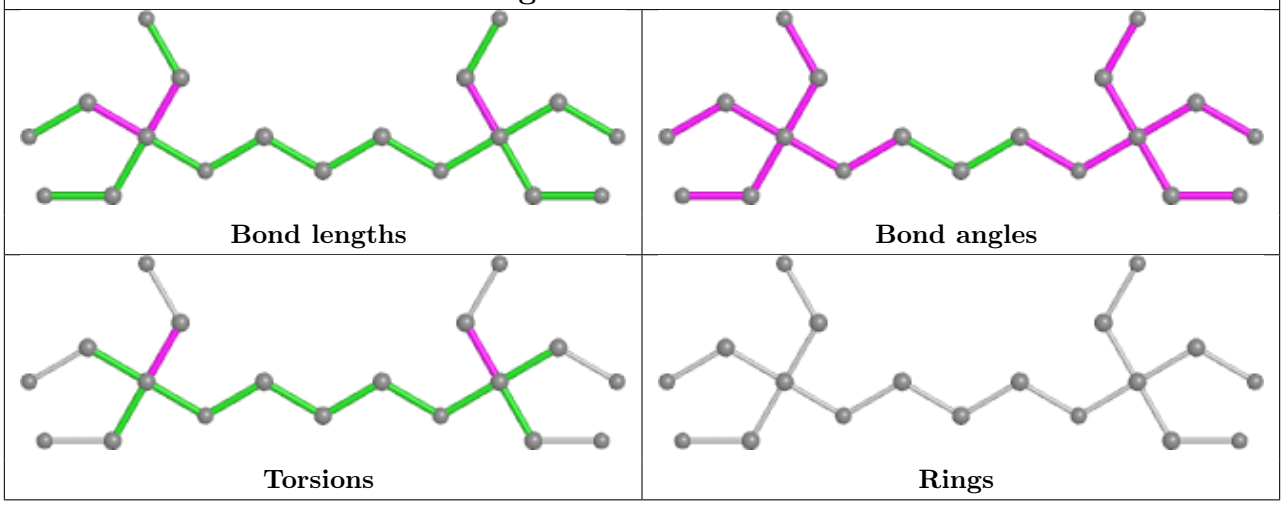
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1434	B3P	3	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.

Ligand B3P K 1434



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%)	-0.11	6 (1%)	75	82	6, 13, 34, 54	0
1	B	426/433 (98%)	-0.11	3 (0%)	87	92	7, 15, 30, 52	1 (0%)
1	C	420/433 (96%)	-0.17	4 (0%)	82	87	6, 14, 29, 59	0
1	D	421/433 (97%)	-0.21	4 (0%)	82	87	6, 14, 26, 58	0
1	E	419/433 (96%)	-0.17	4 (0%)	82	87	6, 13, 30, 53	0
1	F	419/433 (96%)	-0.14	3 (0%)	87	92	6, 14, 26, 69	0
1	G	419/433 (96%)	-0.02	4 (0%)	82	87	9, 17, 32, 56	0
1	H	421/433 (97%)	-0.13	6 (1%)	75	82	8, 15, 29, 53	0
1	I	420/433 (96%)	-0.07	4 (0%)	82	87	8, 15, 29, 57	0
1	J	420/433 (96%)	-0.10	5 (1%)	79	84	6, 16, 29, 67	0
1	K	426/433 (98%)	-0.15	6 (1%)	75	82	6, 14, 29, 67	0
1	L	419/433 (96%)	-0.09	4 (0%)	82	87	7, 14, 29, 56	0
All	All	5055/5196 (97%)	-0.12	53 (1%)	82	87	6, 14, 30, 69	1 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	348	ALA	5.9
1	B	348	ALA	4.6
1	A	405	LEU	4.4
1	J	235	ALA	4.4
1	G	383	ALA	4.1
1	J	236	GLU	4.0
1	D	345	ALA	4.0
1	K	235	ALA	3.6
1	E	86	GLY	3.5
1	C	235	ALA	3.4
1	K	236	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	236	GLU	3.2
1	C	345	ALA	3.2
1	F	236	GLU	3.1
1	F	344	GLY	3.0
1	H	432[A]	ARG	3.0
1	H	346	TYR	2.9
1	L	236	GLU	2.8
1	K	87	PRO	2.7
1	E	344	GLY	2.7
1	F	8	ASP	2.7
1	A	88	LEU	2.6
1	A	416	ASP	2.6
1	B	350	ALA	2.6
1	A	409	GLU	2.6
1	A	235	ALA	2.6
1	J	381	ASP	2.6
1	C	236	GLU	2.5
1	J	345	ALA	2.5
1	I	420	CYS	2.5
1	H	344	GLY	2.4
1	H	88	LEU	2.4
1	A	87	PRO	2.4
1	D	236	GLU	2.4
1	E	352	GLY	2.4
1	G	105	ALA	2.4
1	H	236	GLU	2.3
1	K	349	LYS	2.3
1	L	379	ALA	2.3
1	E	87	PRO	2.3
1	L	372	GLU	2.2
1	H	433	ARG	2.2
1	I	419	SER	2.2
1	D	235	ALA	2.2
1	J	318	TRP	2.1
1	G	236	GLU	2.1
1	B	107	PRO	2.1
1	G	389	ASN	2.1
1	K	382	LEU	2.1
1	D	344	GLY	2.1
1	C	88	LEU	2.1
1	I	416	ASP	2.1
1	L	411	PRO	2.1

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)

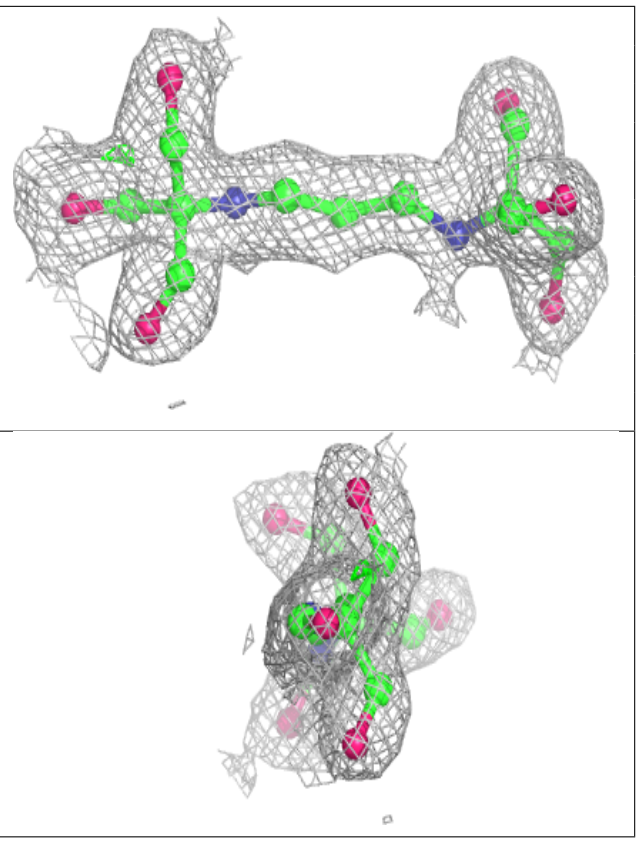
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	B3P	K	1434	19/19	0.92	0.10	15,23,32,33	0
2	FE	J	800	1/1	0.99	0.03	13,13,13,13	0
2	FE	C	800	1/1	1.00	0.04	8,8,8,8	0
2	FE	D	800	1/1	1.00	0.04	9,9,9,9	0
2	FE	E	800	1/1	1.00	0.03	11,11,11,11	0
2	FE	F	800	1/1	1.00	0.06	10,10,10,10	0
2	FE	G	800	1/1	1.00	0.06	12,12,12,12	0
2	FE	H	800	1/1	1.00	0.04	13,13,13,13	0
2	FE	I	800	1/1	1.00	0.04	15,15,15,15	0
2	FE	A	800	1/1	1.00	0.03	14,14,14,14	0
2	FE	K	800	1/1	1.00	0.04	10,10,10,10	0
2	FE	L	800	1/1	1.00	0.07	12,12,12,12	0
2	FE	B	800	1/1	1.00	0.04	12,12,12,12	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 1434:

$2mF_o$-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.