



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:54 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) 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

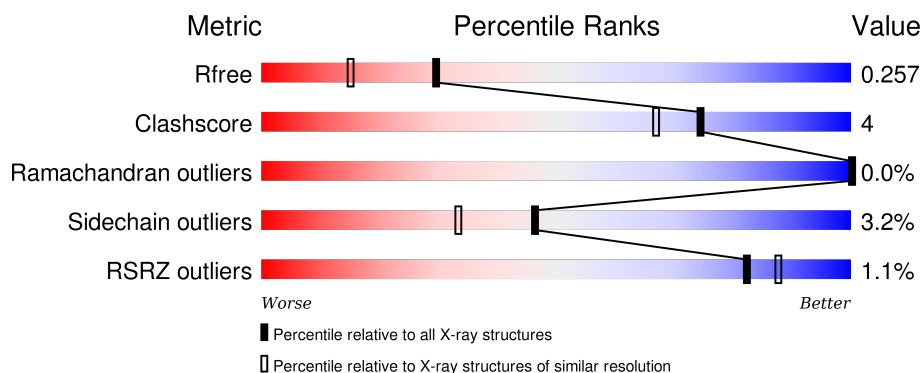
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>..</div> </div> </div>
1	B	433	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>.</div> </div> </div>
1	C	433	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>.</div> </div> </div>
1	D	433	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>..</div> </div> </div>
1	E	433	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>..</div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	433	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>86%</div><div>9%</div><div><div></div><div></div></div></div></div>
1	G	433	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>86%</div><div>10%</div><div><div></div><div></div></div></div></div>
1	H	433	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>88%</div><div>9%</div><div><div></div><div></div></div></div></div>
1	I	433	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>86%</div><div>11%</div><div><div></div><div></div></div></div></div>
1	J	433	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>86%</div><div>10%</div><div><div></div><div></div></div></div></div>
1	K	433	<div><div><div>2%</div><div><div></div><div></div><div></div></div><div>87%</div><div>11%</div><div><div></div><div></div></div></div></div>
1	L	433	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>86%</div><div>11%</div><div><div></div><div></div></div></div></div>

## 2 Entry composition

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 HOMOGENITISATE 1,2-DIOXYGENASE.

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

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

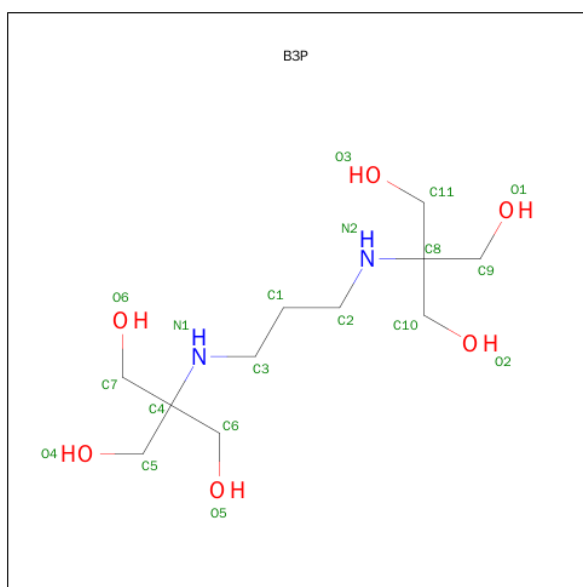
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Fe	0	0
			1	1		
2	J	1	Total	Fe	0	0
			1	1		

*Continued on next page...*

Continued from previous page...

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

- 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
3	K	1	Total	C	N	O	0	0
			19	11	2	6		

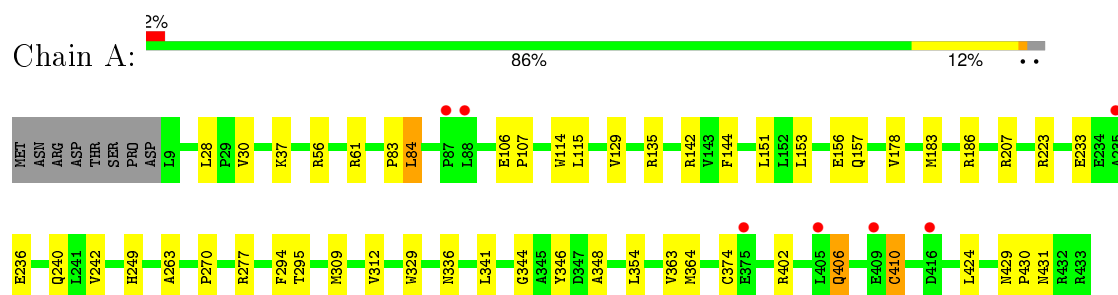
- Molecule 4 is water.

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

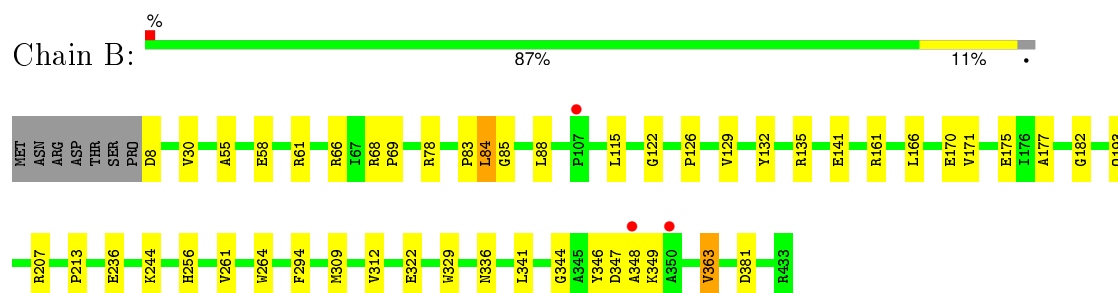
### 3 Residue-property plots

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.

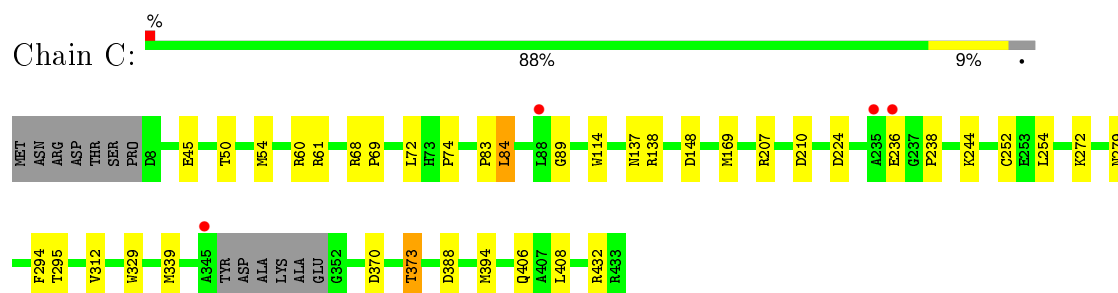
#### • Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE



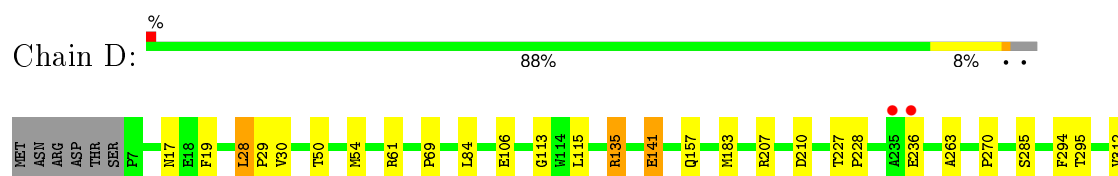
#### • Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

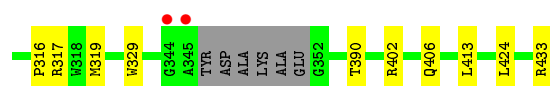


#### • Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

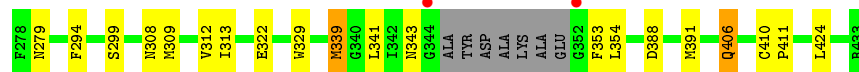
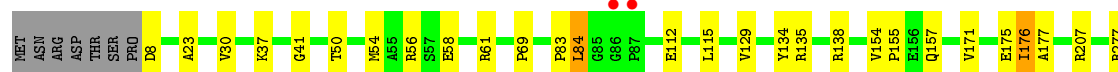
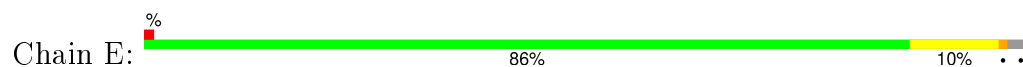


#### • Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE

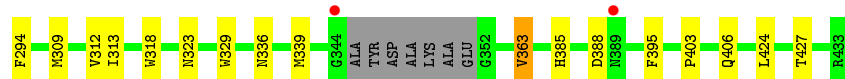
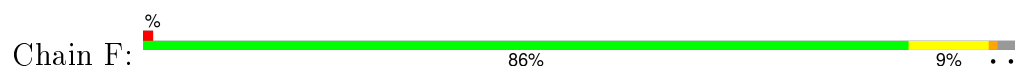




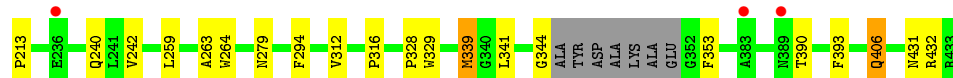
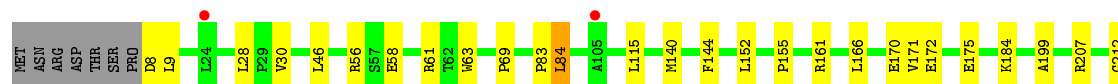
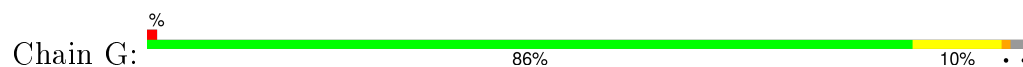
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE



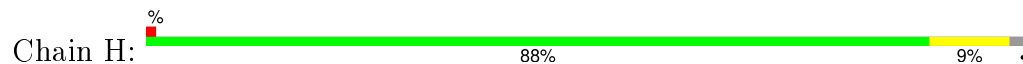
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE



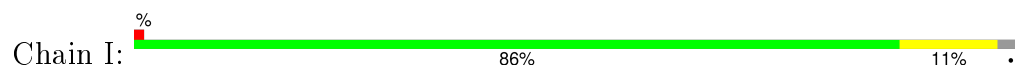
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE



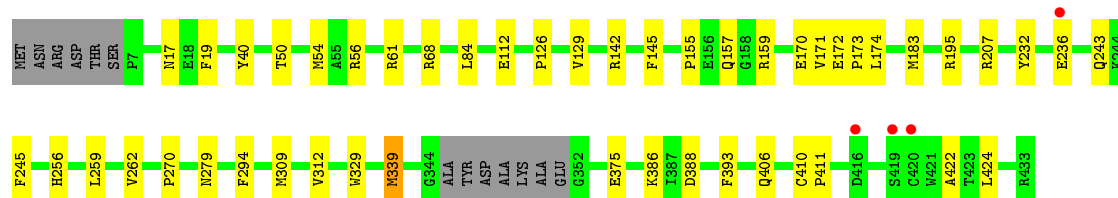
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE



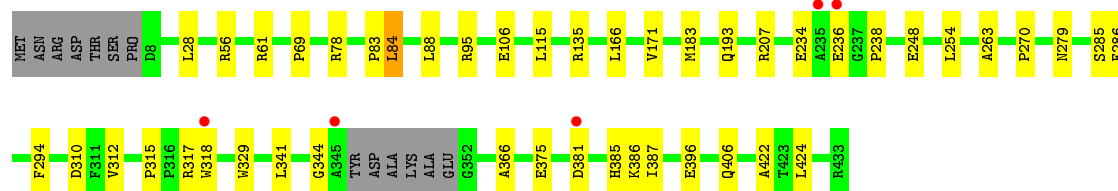
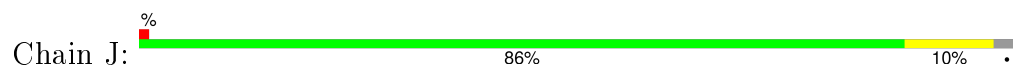
• Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE



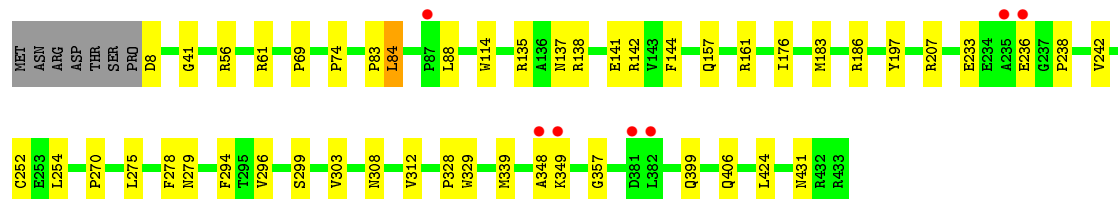
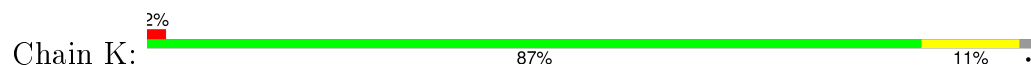




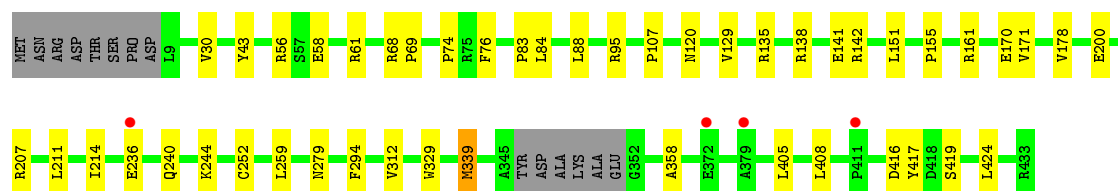
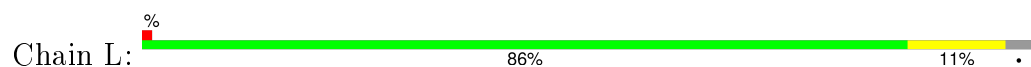
• Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE



• Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE



• Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 94.3 (34.31-1.95)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 1.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.193 , 0.257 0.193 , 0.257	Depositor DCC
$R_{free}$ test set	17580 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 66.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 351613 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	45534	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: 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

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

*Continued on next page...*

*Continued from previous page...*

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:CD	1:H:56:ARG:CB	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:E:83:PRO:HB2	1:E:84:LEU:HD13	1.78	0.65
1:B:55:ALA:HB3	1:B:58[A]:GLU:HG3	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:G:432[A]:ARG:NH1	4:G:2463:HOH:O	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:B:83:PRO:HB2	1:B:84:LEU:HD13	1.82	0.62

Continued on next page...

*Continued from previous page...*

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:L:74:PRO:HG2	1:L:252:CYS:HB2	1.83	0.60
1:K:157:GLN:NE2	4:K:2244:HOH:O	2.32	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:L:294:PHE:HB2	1:L:312:VAL:HG13	1.85	0.59
1:K:142:ARG:HD3	3:K:1434:B3P:H51	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:K:431:ASN:O	4:K:2434:HOH:O	2.17	0.57
1:J:375:GLU:OE2	4:J:2406: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:L:200:GLU:OE2	1:L:244:LYS:NZ	2.34	0.56
1:K:176:ILE:N	4:K:2259:HOH:O	2.38	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:G:432[B]:ARG:NH2	4:G:2466:HOH:O	2.38	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
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

*Continued on next page...*

*Continued from previous page...*

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: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
1:B:193:GLN:OE1	4:B:2303:HOH:O	2.18	0.54
4:J:2166:HOH:O	1:L:76:PHE:O	2.18	0.54
1:A:153:LEU:HG	4:A:2277:HOH:O	2.07	0.54
1:A:56:ARG:NH2	4:A:2112:HOH:O	2.21	0.54
1:K:186:ARG:NH2	1:K:233:GLU:OE2	2.26	0.54
1:L:405:LEU:O	4:L:2376:HOH:O	2.18	0.54
1:I:183:MET:SD	1:I:270:PRO:HD3	2.47	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:B:347:ASP:HB3	4:B:2406:HOH:O	2.08	0.53
1:A:142:ARG:HD3	1:A:240:GLN:OE1	2.09	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:K:83:PRO:HB2	1:K:84:LEU:HD13	1.91	0.52
1:H:379:ALA:O	4:H:2466:HOH:O	2.19	0.52
1:E:277:ARG:NH1	4:E:2325:HOH:O	2.42	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:E:112:GLU:O	4:E:2155:HOH:O	2.19	0.51
1:L:58:GLU:OE1	4:L:2083:HOH:O	2.19	0.51
1:A:84:LEU:HD11	1:A:114:TRP:HB2	1.93	0.51
1:F:135:ARG:NH2	4:F:2176:HOH:O	2.43	0.51
1:F:114:TRP:HH2	4:F:2234:HOH:O	1.93	0.51
1:J:424:LEU:HD13	1:L:69:PRO:HG2	1.91	0.51
1:G:339:MET:HE3	1:G:393:PHE:O	2.10	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:D:183:MET:SD	1:D:270:PRO:HD3	2.52	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:PHE:HB2	1:B:312:VAL:HG13	1.92	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:K:275:LEU:HG	4:K:2259:HOH:O	2.11	0.50
1:D:50:THR:HB	1:D:54:MET:HG3	1.92	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
4:E:2063:HOH:O	1:F:323:ASN:HB3	2.13	0.48
1:E:157:GLN:OE1	4:E:2267:HOH:O	2.19	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:CD	1:G:406:GLN:H	2.17	0.48
1:F:101:GLN:NE2	4:F:2162:HOH:O	2.46	0.48
1:C:45:GLU:HG2	4:C:2075:HOH:O	2.13	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:J:234:GLU:OE2	4:J:2315:HOH:O	2.20	0.47
1:E:37:LYS:HA	4:E:2072:HOH:O	2.14	0.47
1:F:8:ASP:N	1:F:8:ASP:OD1	2.48	0.47
1:C:295:THR:HA	1:C:312:VAL:HG22	1.95	0.47
1:F:8:ASP:HB3	4:F:2004:HOH:O	2.15	0.47
1:E:50:THR:HB	1:E:54:MET:HG3	1.95	0.47
1:C:339:MET:HG2	1:C:394:MET:HB2	1.97	0.47
1:E:406:GLN:H	1:E:406:GLN:CD	2.18	0.47
1:B:126:PRO:HA	4:B:2219:HOH:O	2.14	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

*Continued on next page...*



*Continued from previous page...*

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:J:69:PRO:HG2	1:K:424:LEU:HD13	1.96	0.46
1:F:294:PHE:HB2	1:F:312:VAL:HG13	1.98	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:L:408:LEU:HB2	4:L:2376:HOH:O	2.15	0.46
1:F:102:PRO:O	4:F:2163:HOH:O	2.21	0.46
1:A:277:ARG:NE	4:A:2382:HOH:O	2.49	0.46
4:J:2352:HOH:O	1:K:303:VAL:HG22	2.14	0.46
1:C:68:ARG:HD3	1:C:72:LEU:HD23	1.96	0.46
1:K:299:SER:O	1:K:308:ASN:N	2.49	0.46
1:D:433:ARG:NH2	4:D:2469:HOH:O	2.48	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
1:F:84:LEU:HD11	1:F:114:TRP:HB2	1.98	0.45
1:K:141:GLU:OE1	3:K:1434:B3P:N2	2.49	0.45
1:G:152:LEU:HB3	1:G:199:ALA:HB3	1.99	0.45
4:C:2182:HOH:O	1:D:285:SER:HB2	2.16	0.45
1:A:156:GLU:OE2	1:A:157:GLN:HG3	2.17	0.45
1:L:83:PRO:HG2	1:L:84:LEU:HD13	1.98	0.45
1:G:144:PHE:HA	1:G:242:VAL:O	2.16	0.45
1:B:341:LEU:HD21	1:B:344:GLY:O	2.16	0.45
1:B:166:LEU:HD13	1:B:264:TRP:CD2	2.52	0.45
1:H:93:PRO:HB3	1:I:245:PHE:CG	2.51	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:151:LEU:O	1:H:178:VAL:HA	2.17	0.45
1:J:238:PRO:HA	1:J:254:LEU:O	2.17	0.45
1:I:68:ARG:HD2	1:I:256:HIS:CG	2.52	0.45
1:L:142:ARG:HD3	1:L:240:GLN:OE1	2.17	0.44
1:K:137:ASN:OD1	1:K:138:ARG:HG2	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:D:17:ASN:HB2	1:D:19:PHE:CZ	2.53	0.44
1:G:328:PRO:HD3	4:G:2357:HOH:O	2.16	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:151:LEU:O	1:L:178:VAL:HA	2.17	0.44
1:A:144:PHE:HA	1:A:242:VAL:O	2.17	0.44
1:D:106:GLU:HG3	4:D:2189: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:E:134:TYR:HB2	4:E:2204:HOH: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:I:410:CYS:HA	1:I:411:PRO:HD3	1.82	0.43
1:G:316:PRO:HD3	1:G:390:THR:O	2.18	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:H:433:ARG:HD2	4:H:2525:HOH:O	2.18	0.43
1:G:155:PRO:HD2	1:G:175:GLU:O	2.19	0.43
4:H:2318:HOH:O	1:K:56:ARG:NH2	2.30	0.43
1:F:58[B]:GLU:OE1	1:F:207:ARG:NH1	2.43	0.43
1:I:17:ASN:HB2	1:I:19:PHE:CZ	2.54	0.43
1:H:68:ARG:NH2	4:H:2137:HOH:O	2.51	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:I:126:PRO:HA	4:I:2194:HOH:O	2.17	0.42
1:F:129:VAL:HG21	1:F:309:MET:HB3	2.01	0.42
1:K:339:MET:HB3	1:K:339:MET:HE2	1.89	0.42
1:G:161:ARG:NH2	4:G:2260:HOH:O	2.41	0.42
1:J:315:PRO:O	1:J:317:ARG:NH1	2.50	0.42
1:A:106[A]:GLU:HG3	1:A:107:PRO:HD2	2.02	0.42
1:G:212:GLY:HA3	1:G:213:PRO:HD3	1.84	0.42
1:F:238:PRO:HA	1:F:254:LEU: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:B:85:GLY:HA2	4:B:2165:HOH:O	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

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:232:TYR:CD1	1:I:262:VAL:HG22	2.55	0.42
1:I:170:GLU:OE1	4:I:2250:HOH:O	2.22	0.42
1:K:238:PRO:HA	1:K:254:LEU:O	2.19	0.42
1:K:144:PHE:HA	1:K:242:VAL:O	2.20	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:A:37:LYS:HA	4:A:2069:HOH:O	2.19	0.42
1:I:155:PRO:HG2	1:I:171:VAL:HG12	2.01	0.42
1:E:41:GLY:O	1:F:427:THR:OG1	2.30	0.42
1:E:138:ARG:NH1	4:E:2239:HOH:O	2.52	0.42
1:A:341:LEU:HD21	1:A:344:GLY:O	2.20	0.42
1:A:431:ASN:ND2	4:A:2507:HOH:O	2.52	0.42
1:A:346:TYR:CE2	1:A:348:ALA:HB3	2.54	0.42
1:F:131:ILE:HD13	1:F:395:PHE:HD2	1.85	0.42
1:A:83:PRO:HG2	1:A:249:HIS:CE1	2.54	0.42
1:A:183:MET:SD	1:A:270:PRO:HD3	2.59	0.41
1:D:316:PRO:HD3	1:D:390:THR:O	2.20	0.41
1:C:406:GLN:NE2	4:C:2142:HOH:O	2.53	0.41
1:H:373[A]:THR:HG23	4:H:2454:HOH:O	2.21	0.41
1:F:403:PRO:HD2	4:F:2134:HOH:O	2.20	0.41
4:A:2350:HOH:O	1:D:29:PRO:O	2.22	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:C:137:ASN:O	1:C:138:ARG:HD3	2.21	0.41
1:B:68:ARG:HD2	1:B:256:HIS:CG	2.55	0.41
1:A:336:ASN:OD1	1:A:363:VAL:HG23	2.20	0.41
3:K:1434:B3P:H52	3:K:1434:B3P:H32	1.86	0.41
1:K:278:PHE:CE1	1:K:296:VAL:HG22	2.55	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:H:68:ARG:HD2	1:H:256:HIS:CG	2.56	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:B:78:ARG:NH2	4:B:2155:HOH:O	2.36	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:K:339:MET:HG3	4:K:2368:HOH:O	2.20	0.41
1:H:372:GLU:HB3	4:H:2454:HOH:O	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:385:HIS:HB2	4:F:2389:HOH:O	2.21	0.41
1:J:183:MET:SD	1:J:270:PRO:HD3	2.60	0.41
1:G:166:LEU:HB3	1:G:264:TRP:CE2	2.56	0.41
1:I:145:PHE:O	1:I:243:GLN:HA	2.20	0.41
1:L:155:PRO:HG2	1:L:171:VAL:HG12	2.02	0.41
1:H:95:ARG:HD3	1:H:366:ALA:O	2.20	0.41
1:E:410:CYS:HA	1:E:411:PRO:HD3	1.92	0.41
1:J:341:LEU:HD21	1:J:344:GLY:O	2.20	0.41
1:H:294:PHE:HB2	1:H:312:VAL:HG13	2.03	0.41
1:L:416:ASP:O	1:L:419:SER:OG	2.37	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:B:171:VAL:HG21	1:B:177:ALA:HB2	2.03	0.41
1:E:339:MET:HB3	1:E:339:MET:HE2	1.92	0.41
1:B:66:ARG:HB3	1:B:261:VAL:HG22	2.03	0.40
1:L:417:TYR:HA	4:L:2144:HOH:O	2.21	0.40
1:C:210:ASP:HB2	4:C:2298:HOH:O	2.20	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:H:82:GLN:HA	4:H:2155:HOH:O	2.20	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:A:151:LEU:O	1:A:178:VAL:HA	2.21	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
1:E:154:VAL:HG22	1:E:176:ILE:HG22	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%)	34	21
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%)	34	21
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	48

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 ⓘ

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%)	46	33
1	B	350/355 (99%)	340 (97%)	10 (3%)	50	38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	347/355 (98%)	338 (97%)	9 (3%)	54	43
1	D	346/355 (98%)	335 (97%)	11 (3%)	46	33
1	E	343/355 (97%)	328 (96%)	15 (4%)	35	19
1	F	345/355 (97%)	336 (97%)	9 (3%)	54	43
1	G	346/355 (98%)	332 (96%)	14 (4%)	38	23
1	H	349/355 (98%)	339 (97%)	10 (3%)	50	38
1	I	344/355 (97%)	334 (97%)	10 (3%)	50	38
1	J	344/355 (97%)	331 (96%)	13 (4%)	40	25
1	K	348/355 (98%)	338 (97%)	10 (3%)	50	38
1	L	344/355 (97%)	333 (97%)	11 (3%)	46	33
All	All	4155/4260 (98%)	4022 (97%)	133 (3%)	46	33

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

Some 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

*Continued on next page...*

*Continued from previous page...*

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 carbohydrates 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	1.56	3 (16%)	23,23,23	1.73	8 (34%)

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	-	-	0/28/28/28	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1434	B3P	C5-C4	-3.91	1.49	1.53
3	K	1434	B3P	C6-C4	-2.41	1.50	1.53
3	K	1434	B3P	C11-C8	-2.15	1.51	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1434	B3P	C2-N2-C8	-3.21	111.28	116.07
3	K	1434	B3P	C3-N1-C4	-2.03	113.03	116.07
3	K	1434	B3P	O4-C5-C4	2.06	115.70	111.42
3	K	1434	B3P	O5-C6-C4	2.32	116.24	111.42
3	K	1434	B3P	O2-C10-C8	2.74	117.11	111.42
3	K	1434	B3P	O1-C9-C8	2.94	117.53	111.42
3	K	1434	B3P	O6-C7-C4	2.98	117.61	111.42
3	K	1434	B3P	O3-C11-C8	3.28	118.23	111.42

There are no chirality outliers.

There are no torsion outliers.

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

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	425/433 (98%)	-0.08	7 (1%) 74 83	6, 13, 34, 54	0
1	B	426/433 (98%)	-0.07	3 (0%) 89 93	7, 15, 30, 52	1 (0%)
1	C	420/433 (96%)	-0.14	4 (0%) 84 89	6, 14, 29, 59	0
1	D	421/433 (97%)	-0.18	4 (0%) 84 89	6, 14, 26, 58	0
1	E	419/433 (96%)	-0.14	4 (0%) 84 89	6, 13, 30, 53	0
1	F	419/433 (96%)	-0.11	4 (0%) 84 89	6, 14, 26, 69	0
1	G	419/433 (96%)	0.01	5 (1%) 81 87	9, 17, 32, 56	0
1	H	421/433 (97%)	-0.09	6 (1%) 78 85	8, 15, 29, 53	0
1	I	420/433 (96%)	-0.04	4 (0%) 84 89	8, 15, 29, 57	0
1	J	420/433 (96%)	-0.07	5 (1%) 81 87	6, 16, 29, 67	0
1	K	426/433 (98%)	-0.11	7 (1%) 74 83	6, 14, 29, 67	0
1	L	419/433 (96%)	-0.06	4 (0%) 84 89	7, 14, 29, 56	0
All	All	5055/5196 (97%)	-0.09	57 (1%) 82 88	6, 14, 30, 69	1 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	348	ALA	6.1
1	B	348	ALA	4.6
1	A	405	LEU	4.5
1	J	235	ALA	4.4
1	G	383	ALA	4.2
1	D	345	ALA	4.1
1	J	236	GLU	4.1
1	K	235	ALA	3.7
1	C	235	ALA	3.6
1	E	86	GLY	3.6
1	K	236	GLU	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	236	GLU	3.3
1	C	345	ALA	3.3
1	F	236	GLU	3.1
1	F	344	GLY	3.1
1	H	432[A]	ARG	3.0
1	H	346	TYR	3.0
1	L	236	GLU	2.9
1	K	87	PRO	2.7
1	A	88	LEU	2.7
1	E	344	GLY	2.7
1	A	416	ASP	2.7
1	F	8	ASP	2.7
1	A	409	GLU	2.6
1	J	381	ASP	2.6
1	A	235	ALA	2.6
1	B	350	ALA	2.6
1	I	420	CYS	2.6
1	C	236	GLU	2.6
1	J	345	ALA	2.6
1	H	88	LEU	2.5
1	H	344	GLY	2.5
1	G	105	ALA	2.4
1	E	352	GLY	2.4
1	D	236	GLU	2.4
1	A	87	PRO	2.4
1	E	87	PRO	2.4
1	L	379	ALA	2.4
1	H	236	GLU	2.3
1	K	349	LYS	2.3
1	L	372	GLU	2.3
1	H	433	ARG	2.2
1	D	235	ALA	2.2
1	J	318	TRP	2.2
1	I	419	SER	2.2
1	K	382	LEU	2.2
1	G	236	GLU	2.2
1	G	389	ASN	2.2
1	I	416	ASP	2.2
1	B	107	PRO	2.1
1	D	344	GLY	2.1
1	L	411	PRO	2.1
1	G	24	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	88	LEU	2.0
1	K	381	ASP	2.0
1	A	375	GLU	2.0
1	F	389	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 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	B3P	K	1434	19/19	0.91	0.10	1.02	15,23,32,33	0
2	FE	H	800	1/1	1.00	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	A	800	1/1	1.00	0.03	-	14,14,14,14	0
2	FE	B	800	1/1	1.00	0.04	-	12,12,12,12	0
2	FE	G	800	1/1	1.00	0.06	-	12,12,12,12	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	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	I	800	1/1	1.00	0.04	-	15,15,15,15	0
2	FE	J	800	1/1	0.99	0.03	-	13,13,13,13	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.