



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:13 PM GMT

PDB ID : 4KWF
Title : Crystal Structure Analysis of ALDH2+ALDiB33
Authors : Hurley, T.D.; Kimble-Hill, A.C.
Deposited on : 2013-05-24
Resolution : 2.31 Å(reported)

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

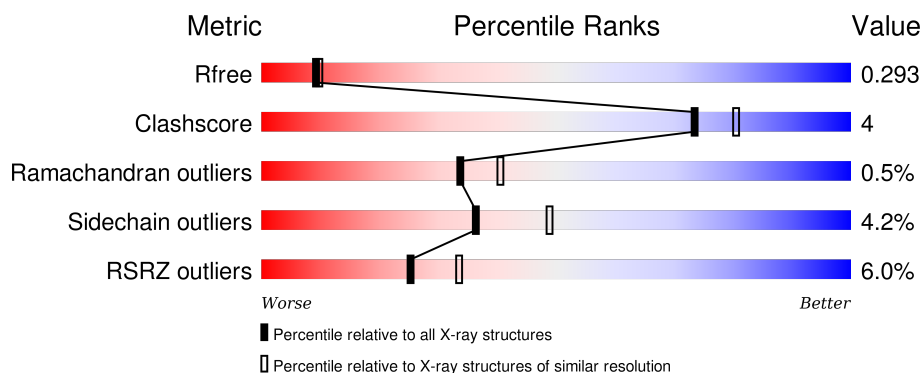
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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.



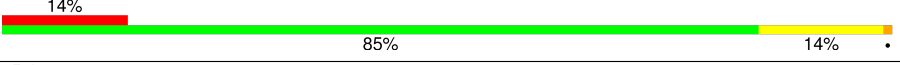


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	494	<div> <div>5%</div> <div>89%</div> <div>10%</div> </div>
1	B	494	<div> <div>12%</div> <div>85%</div> <div>13%</div> </div>
1	C	494	<div> <div>5%</div> <div>89%</div> <div>10%</div> </div>
1	D	494	<div> <div>2%</div> <div>89%</div> <div>11%</div> </div>
1	E	494	<div> <div>4%</div> <div>86%</div> <div>14%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	494	
1	G	494	
1	H	494	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3AK	B	601	-	-	X	-
3	NA	A	602	-	-	-	X
3	NA	C	601	-	-	-	X
4	EDO	A	604	-	-	-	X
4	EDO	C	602	-	-	-	X
4	EDO	C	603	-	-	-	X
4	EDO	E	603	-	-	-	X
4	EDO	E	604	-	-	-	X
4	EDO	H	603	-	-	-	X
5	GAI	F	603	-	-	-	X
5	GAI	H	604	-	-	-	X

2 Entry composition

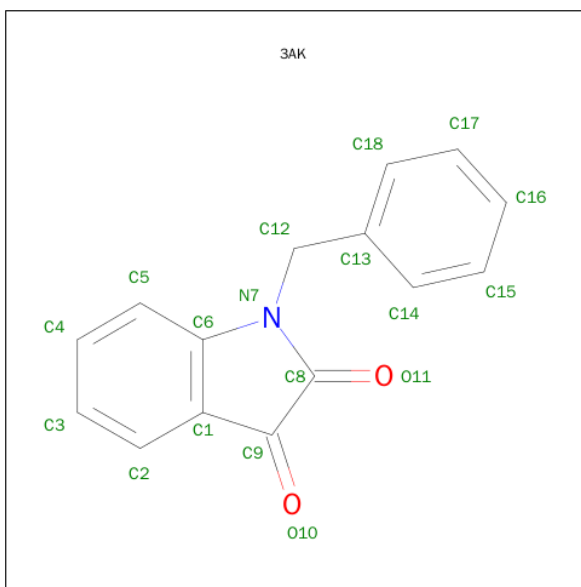
There are 6 unique types of molecules in this entry. The entry contains 30712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aldehyde dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	B	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	C	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	D	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	E	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	F	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	G	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	H	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			

- Molecule 2 is 1-BENZYL-1H-INDOLE-2,3-DIONE (three-letter code: 3AK) (formula: C₁₅H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	15	1	2		
2	B	1	Total	C	N	O	0	0
			18	15	1	2		
2	E	1	Total	C	N	O	0	0
			18	15	1	2		
2	H	1	Total	C	N	O	0	0
			18	15	1	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

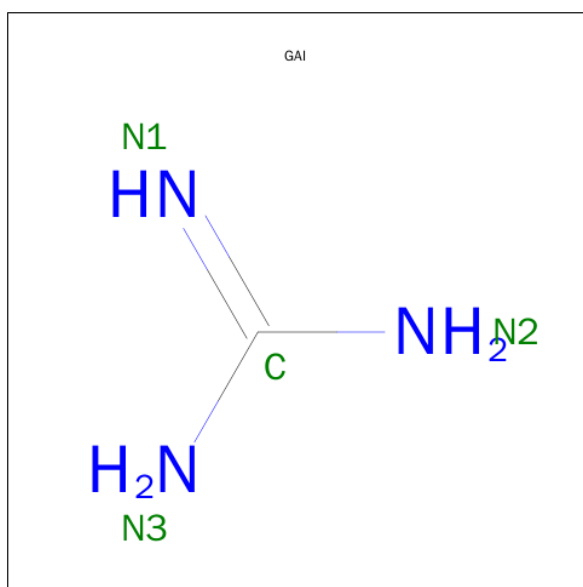
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		
3	H	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
3	F	1	Total	Na	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GUANIDINE (three-letter code: GAI) (formula: CH_5N_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			4	1	3		
5	B	1	Total	C	N	0	0
			4	1	3		
5	C	1	Total	C	N	0	0
			4	1	3		
5	D	1	Total	C	N	0	0
			4	1	3		
5	F	1	Total	C	N	0	0
			4	1	3		
5	G	1	Total	C	N	0	0
			4	1	3		
5	H	1	Total	C	N	0	0
			4	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	24	Total	O	0	0
			24	24		
6	B	15	Total	O	0	0
			15	15		
6	C	17	Total	O	0	0
			17	17		
6	D	31	Total	O	0	0
			31	31		
6	E	20	Total	O	0	0
			20	20		

Continued on next page...

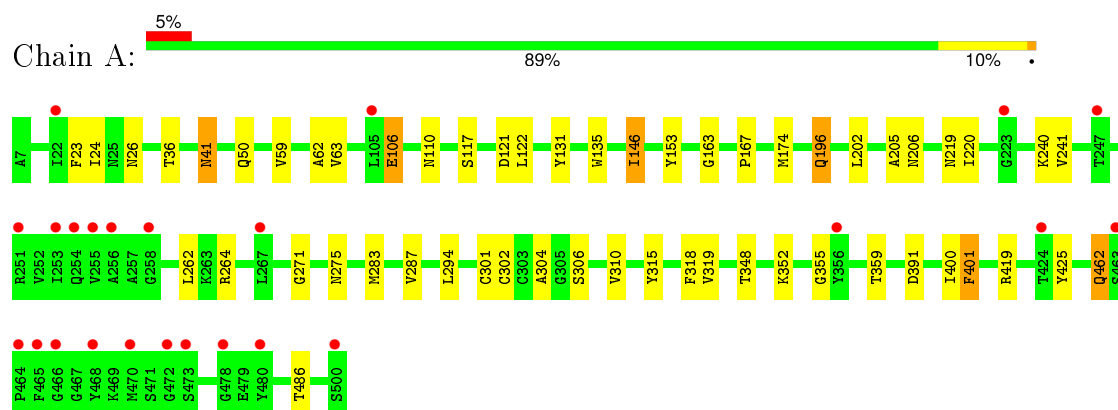
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	20	Total 20	O 20	0	0
6	G	16	Total 16	O 16	0	0
6	H	45	Total 45	O 45	0	0

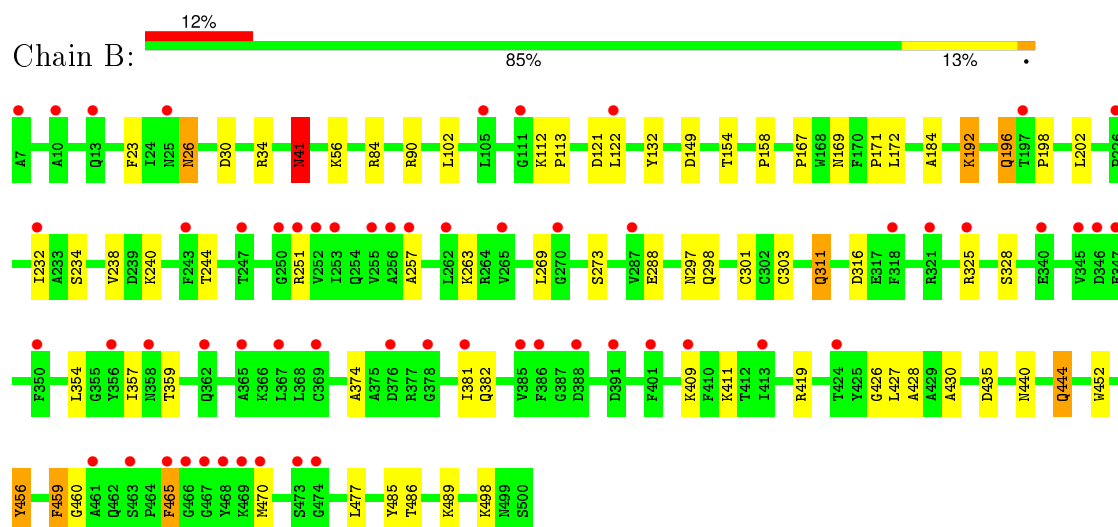
3 Residue-property plots [i](#)

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

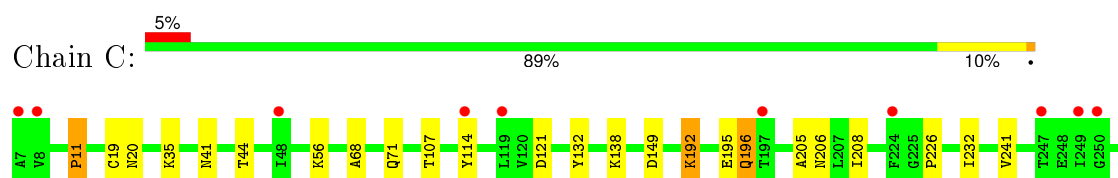
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

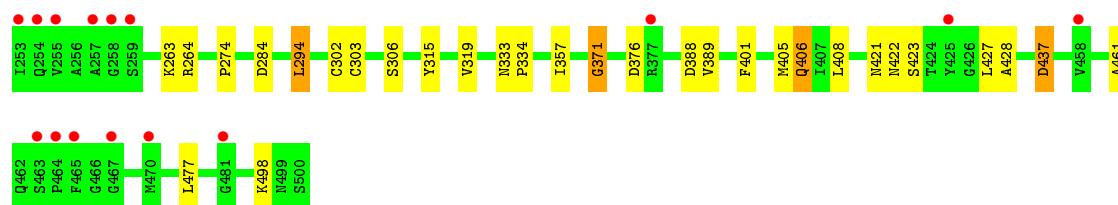


- Molecule 1: Aldehyde dehydrogenase, mitochondrial

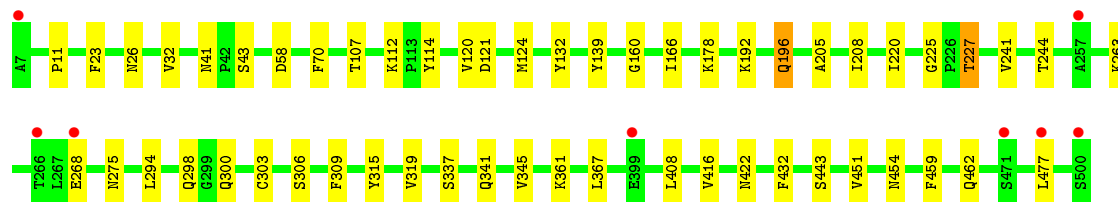
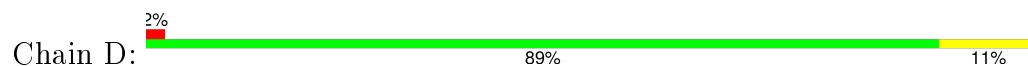


- Molecule 1: Aldehyde dehydrogenase, mitochondrial

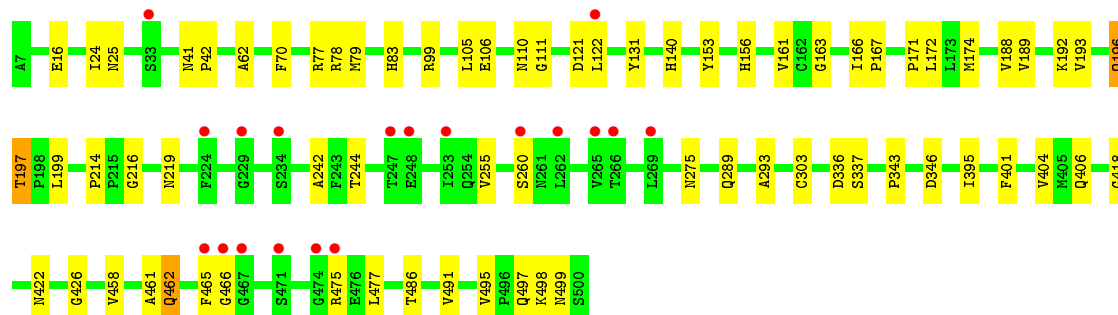
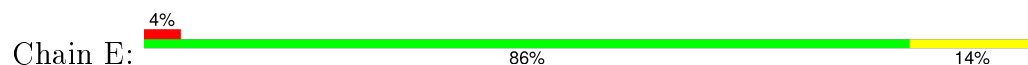




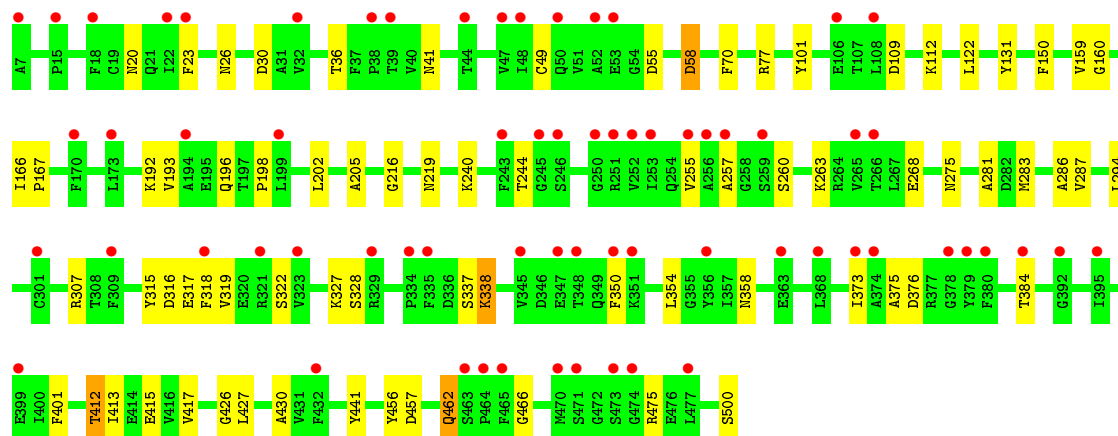
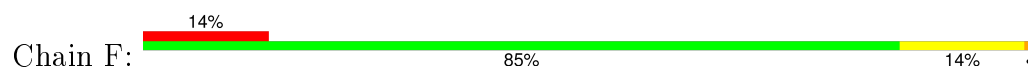
- Molecule 1: Aldehyde dehydrogenase, mitochondrial



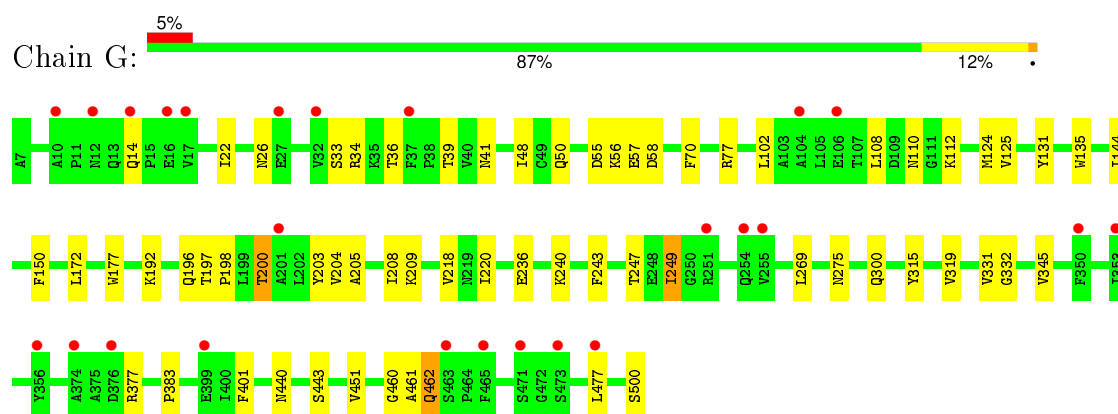
- Molecule 1: Aldehyde dehydrogenase, mitochondrial



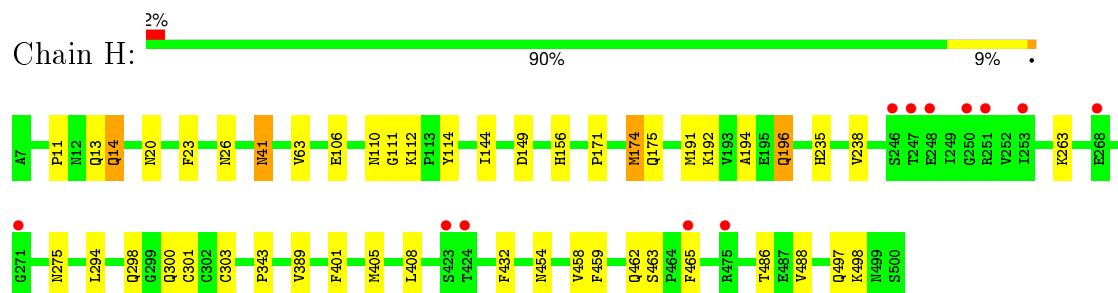
- Molecule 1: Aldehyde dehydrogenase, mitochondrial



- Molecule 1: Aldehyde dehydrogenase, mitochondrial



- Molecule 1: Aldehyde dehydrogenase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.29Å 177.09Å 102.55Å 90.00° 94.39° 90.00°	Depositor
Resolution (Å)	49.12 – 2.31 49.12 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.12-2.31) 98.8 (49.12-2.31)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.239 , 0.296 0.238 , 0.293	Depositor DCC
R_{free} test set	8003 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 20.1	EDS
Estimated twinning fraction	0.277 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	0 of 158309 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30712	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3AK, NA, EDO, GAI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/3882	0.59	0/5267
1	B	0.38	0/3882	0.56	0/5267
1	C	0.40	0/3882	0.57	0/5267
1	D	0.44	0/3882	0.59	0/5267
1	E	0.41	0/3882	0.58	0/5267
1	F	0.37	0/3882	0.56	0/5267
1	G	0.40	0/3882	0.56	0/5267
1	H	0.44	0/3882	0.60	0/5267
All	All	0.41	0/31056	0.58	0/42136

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	3798	0	3745	32	0
1	B	3798	0	3745	40	0
1	C	3798	0	3745	24	0
1	D	3798	0	3745	28	0
1	E	3798	0	3745	36	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3798	0	3745	31	0
1	G	3798	0	3745	36	0
1	H	3798	0	3745	31	0
2	A	18	0	11	3	0
2	B	18	0	11	8	0
2	E	18	0	11	4	0
2	H	18	0	11	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	8	0	12	2	0
4	C	8	0	12	0	0
4	E	8	0	12	0	0
4	F	4	0	6	0	0
4	H	4	0	6	0	0
5	A	4	0	4	0	0
5	B	4	0	4	1	0
5	C	4	0	4	0	0
5	D	4	0	4	0	0
5	F	4	0	4	0	0
5	G	4	0	4	0	0
5	H	4	0	4	0	0
6	A	24	0	0	0	0
6	B	15	0	0	0	0
6	C	17	0	0	0	0
6	D	31	0	0	0	0
6	E	20	0	0	0	0
6	F	20	0	0	0	0
6	G	16	0	0	0	0
6	H	45	0	0	0	0
All	All	30712	0	30080	246	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (246) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:CYS:SG	2:B:601:3AK:O10	2.26	0.93
1:A:205:ALA:HB2	1:A:220:ILE:HD12	1.60	0.84
1:E:303:CYS:SG	2:E:601:3AK:O10	2.43	0.77
1:G:48:ILE:HG21	1:G:108:LEU:HD21	1.69	0.75
1:E:216:GLY:HA2	1:E:219:ASN:HD21	1.54	0.71
1:F:166:ILE:HD11	1:F:193:VAL:HG12	1.71	0.71
1:G:110:ASN:HD22	1:G:197:THR:HG21	1.56	0.70
1:B:102:LEU:HD22	1:B:172:LEU:HD11	1.73	0.69
1:C:205:ALA:HA	1:C:208:ILE:HD12	1.74	0.69
1:B:196:GLN:H	1:B:196:GLN:HE21	1.39	0.69
1:D:132:TYR:OH	1:D:477:LEU:HA	1.93	0.68
1:A:294:LEU:HD12	1:A:306:SER:HA	1.75	0.68
1:B:311:GLN:NE2	1:B:411:LYS:O	2.27	0.68
1:H:196:GLN:HE21	1:H:196:GLN:H	1.39	0.68
1:C:19:CYS:SG	1:C:206:ASN:ND2	2.66	0.67
1:E:255:VAL:HG13	1:F:255:VAL:HG13	1.77	0.67
1:B:427:LEU:HD21	2:B:601:3AK:C16	2.25	0.66
1:B:427:LEU:HD21	2:B:601:3AK:C15	2.26	0.66
1:G:205:ALA:HB2	1:G:220:ILE:HD12	1.78	0.65
1:B:132:TYR:OH	1:B:477:LEU:HA	1.97	0.65
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.32	0.65
1:B:149:ASP:HA	1:B:498:LYS:HB2	1.79	0.65
1:E:465:PHE:CE2	2:E:601:3AK:H12	2.33	0.64
1:F:287:VAL:HG22	1:F:318:PHE:CD1	2.32	0.64
1:A:41:ASN:HD22	1:A:41:ASN:C	2.00	0.64
1:B:440:ASN:O	1:B:444:GLN:HB2	1.97	0.64
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.34	0.63
1:D:205:ALA:HB2	1:D:220:ILE:HD12	1.80	0.62
1:H:175:GLN:HG3	1:H:191:MET:SD	2.40	0.61
1:H:41:ASN:C	1:H:41:ASN:HD22	2.03	0.61
1:E:465:PHE:CD2	2:E:601:3AK:H12	2.36	0.61
1:D:241:VAL:HG23	1:D:263:LYS:HD3	1.82	0.61
1:A:301:CYS:HB3	2:A:601:3AK:O10	2.01	0.61
1:F:77:ARG:NE	1:G:500:SER:OG	2.32	0.61
1:C:294:LEU:HD12	1:C:306:SER:HA	1.83	0.60
1:E:106:GLU:OE1	1:E:171:PRO:HD2	2.01	0.59
1:F:315:TYR:O	1:F:319:VAL:HG23	2.03	0.59
1:E:131:TYR:CE1	1:E:462:GLN:HG3	2.36	0.59
1:D:196:GLN:H	1:D:196:GLN:HE21	1.51	0.58
1:C:315:TYR:O	1:C:319:VAL:HG23	2.02	0.58
1:E:404:VAL:HG12	1:E:406:GLN:HE22	1.68	0.58
1:G:102:LEU:HD21	1:G:203:TYR:HD2	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:SER:HA	1:D:451:VAL:HG11	1.87	0.56
1:C:132:TYR:OH	1:C:477:LEU:HA	2.06	0.56
1:H:106:GLU:OE1	1:H:171:PRO:HD2	2.06	0.56
1:B:269:LEU:HD12	1:B:470:MET:O	2.05	0.56
1:C:149:ASP:HA	1:C:498:LYS:HB2	1.87	0.55
1:C:461:ALA:HA	1:C:477:LEU:HD22	1.88	0.55
1:D:244:THR:HG23	1:D:268:GLU:HB2	1.89	0.55
1:G:131:TYR:CE1	1:G:462:GLN:HG3	2.42	0.55
1:H:465:PHE:CE2	2:H:601:3AK:H12	2.42	0.55
1:H:196:GLN:H	1:H:196:GLN:NE2	2.04	0.55
1:B:112:LYS:HA	1:B:298:GLN:OE1	2.07	0.55
1:A:36:THR:HB	1:A:50:GLN:HG3	1.90	0.54
1:D:294:LEU:HD13	1:D:294:LEU:C	2.28	0.54
1:D:120:VAL:HG12	1:D:124:MET:CE	2.38	0.53
1:C:68:ALA:HA	1:C:71:GLN:HG2	1.89	0.53
1:B:459:PHE:CZ	2:B:601:3AK:C2	2.92	0.53
1:B:169:ASN:O	1:B:297:ASN:ND2	2.40	0.53
1:F:373:ILE:HG22	1:F:375:ALA:O	2.09	0.52
1:B:301:CYS:SG	2:B:601:3AK:C9	2.97	0.52
1:G:208:ILE:HD13	1:G:218:VAL:HG11	1.92	0.52
1:E:166:ILE:HD11	1:E:193:VAL:HG12	1.92	0.52
1:H:465:PHE:CD2	2:H:601:3AK:H12	2.44	0.52
1:A:310:VAL:HG21	1:A:318:PHE:CD2	2.45	0.52
1:B:84:ARG:NH1	1:B:184:ALA:O	2.43	0.51
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.45	0.51
1:C:196:GLN:H	1:C:196:GLN:HE21	1.59	0.51
1:F:281:ALA:HB1	1:F:286:ALA:HB2	1.93	0.51
1:D:294:LEU:HD23	1:D:306:SER:HA	1.93	0.51
1:G:110:ASN:HD22	1:G:197:THR:CG2	2.23	0.51
1:A:301:CYS:HB2	1:A:304:ALA:HB2	1.93	0.50
1:F:167:PRO:HD3	1:F:244:THR:HB	1.93	0.50
1:B:301:CYS:HG	2:B:601:3AK:C9	2.24	0.50
1:G:462:GLN:HE21	1:G:462:GLN:H	1.59	0.50
1:H:11:PRO:HB3	1:H:114:TYR:CZ	2.47	0.50
1:G:462:GLN:HB3	1:H:144:ILE:CG2	2.41	0.49
1:B:303:CYS:HB2	1:B:428:ALA:HB3	1.93	0.49
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.46	0.49
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.48	0.49
1:G:22:ILE:HD13	1:G:58:ASP:OD1	2.13	0.49
1:H:294:LEU:HD13	1:H:405:MET:HA	1.95	0.49
1:G:462:GLN:NE2	1:G:462:GLN:H	2.10	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:ALA:HA	1:D:208:ILE:HD12	1.95	0.49
1:D:432:PHE:CD2	1:D:454:ASN:HA	2.48	0.49
1:E:111:GLY:O	1:E:343:PRO:HD2	2.13	0.48
1:E:497:GLN:HE21	1:E:499:ASN:HD21	1.60	0.48
1:E:336:ASP:OD1	1:E:337:SER:N	2.46	0.48
1:E:395:ILE:HD12	1:E:406:GLN:HE21	1.79	0.48
1:D:300:GLN:HE22	1:D:345:VAL:H	1.61	0.48
1:H:11:PRO:HB3	1:H:114:TYR:CE1	2.48	0.48
1:D:32:VAL:HG23	1:D:58:ASP:OD1	2.13	0.48
1:C:389:VAL:HB	1:C:408:LEU:HG	1.96	0.48
1:E:79:MET:HE3	1:E:83:HIS:HB3	1.96	0.48
1:B:192:LYS:HB2	1:B:232:ILE:CD1	2.44	0.48
1:C:357:ILE:HG21	1:C:371:GLY:O	2.13	0.48
1:G:110:ASN:ND2	1:G:197:THR:HG21	2.26	0.47
1:A:41:ASN:ND2	1:A:41:ASN:C	2.65	0.47
1:E:495:VAL:HG12	1:G:440:ASN:HD22	1.79	0.47
1:C:437:ASP:N	1:C:437:ASP:OD2	2.47	0.47
1:A:146:ILE:CG1	1:B:460:GLY:HA3	2.45	0.47
1:A:153:TYR:HH	4:A:603:EDO:HO1	1.61	0.47
1:F:430:ALA:HB2	1:F:456:TYR:CD1	2.50	0.47
1:F:216:GLY:O	1:F:219:ASN:ND2	2.47	0.47
1:F:466:GLY:HA3	1:F:475:ARG:HD3	1.97	0.47
1:A:205:ALA:HB2	1:A:220:ILE:CD1	2.40	0.47
1:G:36:THR:OG1	1:G:50:GLN:NE2	2.47	0.47
1:E:466:GLY:HA3	1:E:475:ARG:HD3	1.97	0.47
1:A:355:GLY:O	1:A:359:THR:HG23	2.14	0.47
1:H:174:MET:HE1	2:H:601:3AK:C18	2.45	0.47
1:F:281:ALA:HB1	1:F:286:ALA:CB	2.45	0.47
1:G:460:GLY:O	1:G:462:GLN:N	2.48	0.47
1:A:315:TYR:O	1:A:319:VAL:HG23	2.15	0.46
1:E:24:ILE:HG23	1:E:62:ALA:HA	1.96	0.46
1:D:70:PHE:CE1	1:D:160:GLY:HA2	2.50	0.46
1:A:23:PHE:O	1:A:24:ILE:HG13	2.15	0.46
1:B:167:PRO:HG3	1:B:244:THR:HG22	1.97	0.46
1:C:107:THR:OG1	1:C:114:TYR:HA	2.15	0.46
1:F:287:VAL:HG22	1:F:318:PHE:CE1	2.51	0.46
1:B:41:ASN:HD22	1:B:41:ASN:C	2.18	0.46
1:D:303:CYS:HG	1:D:459:PHE:HZ	1.64	0.46
1:G:26:ASN:HB3	1:G:209:LYS:HE2	1.97	0.46
1:E:346:ASP:OD1	1:E:346:ASP:C	2.54	0.46
1:E:41:ASN:HD22	1:E:42:PRO:HD2	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:O	1:A:205:ALA:HB3	2.15	0.46
1:E:465:PHE:CE2	2:E:601:3AK:C15	2.98	0.46
2:A:601:3AK:O11	2:A:601:3AK:C13	2.64	0.46
1:H:301:CYS:HB3	2:H:601:3AK:O10	2.16	0.46
1:A:106:GLU:O	1:A:110:ASN:HB3	2.15	0.46
1:H:432:PHE:HA	1:H:454:ASN:OD1	2.15	0.46
1:E:105:LEU:HD11	1:E:199:LEU:HD13	1.98	0.46
1:D:11:PRO:HB3	1:D:114:TYR:CZ	2.51	0.46
1:A:135:TRP:CD1	1:C:138:LYS:HE3	2.51	0.46
1:B:374:ALA:HB2	1:B:382:GLN:N	2.31	0.45
1:E:163:GLY:O	1:E:242:ALA:N	2.43	0.45
1:B:409:LYS:O	1:B:419:ARG:NH2	2.46	0.45
1:E:167:PRO:HD3	1:E:244:THR:HB	1.98	0.45
1:G:443:SER:HA	1:G:451:VAL:HG11	1.97	0.45
1:D:309:PHE:CD2	1:D:416:VAL:HG23	2.52	0.45
1:A:294:LEU:CD1	1:A:306:SER:HA	2.43	0.45
1:D:408:LEU:HD12	1:D:408:LEU:N	2.32	0.45
1:F:70:PHE:CZ	1:F:160:GLY:HA2	2.52	0.45
1:H:238:VAL:O	1:H:263:LYS:HE3	2.17	0.45
1:F:412:THR:OG1	1:F:415:GLU:HB2	2.16	0.45
1:B:238:VAL:O	1:B:263:LYS:HE3	2.17	0.45
1:E:418:GLY:O	1:E:422:ASN:HB2	2.16	0.45
1:D:107:THR:HG23	1:D:112:LYS:O	2.17	0.45
1:A:302:CYS:HB2	2:A:601:3AK:O11	2.17	0.44
1:F:101:TYR:C	1:F:101:TYR:CD1	2.91	0.44
1:C:107:THR:HG23	1:C:334:PRO:HB2	1.98	0.44
1:E:196:GLN:H	1:E:196:GLN:HE21	1.65	0.44
1:H:298:GLN:O	1:H:300:GLN:HG3	2.18	0.44
1:B:354:LEU:HA	1:B:357:ILE:HD12	1.99	0.44
1:F:294:LEU:HD13	1:F:294:LEU:C	2.38	0.44
1:A:163:GLY:O	1:A:241:VAL:HA	2.17	0.44
1:D:432:PHE:CE2	1:D:454:ASN:HA	2.53	0.44
1:A:196:GLN:H	1:A:196:GLN:NE2	2.16	0.44
1:D:120:VAL:HG12	1:D:124:MET:HE2	2.00	0.44
1:G:461:ALA:HA	1:G:477:LEU:HD22	1.98	0.44
1:B:459:PHE:CE1	2:B:601:3AK:C3	3.00	0.43
1:A:131:TYR:CE1	1:A:462:GLN:HG3	2.52	0.43
1:F:413:ILE:HG12	1:F:441:TYR:CE2	2.53	0.43
1:A:391:ASP:OD2	1:A:419:ARG:HD2	2.17	0.43
1:H:14:GLN:HB2	1:H:14:GLN:HE21	1.64	0.43
1:B:465:PHE:CE2	2:B:601:3AK:H13	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ALA:HB1	1:B:263:LYS:HG3	2.00	0.43
1:D:166:ILE:HG22	1:D:178:LYS:HD2	1.99	0.43
1:F:350:PHE:CZ	1:F:354:LEU:HD11	2.53	0.43
1:C:315:TYR:HH	1:C:388:ASP:H	1.64	0.43
1:C:192:LYS:HB2	1:C:232:ILE:CD1	2.49	0.43
1:G:243:PHE:CZ	1:G:249:ILE:HB	2.53	0.43
1:H:156:HIS:CD2	1:H:488:VAL:HG22	2.53	0.43
1:C:406:GLN:HE21	1:C:406:GLN:HB2	1.67	0.43
1:H:106:GLU:O	1:H:110:ASN:HB3	2.19	0.43
1:D:120:VAL:HG12	1:D:124:MET:HE1	2.00	0.43
1:B:430:ALA:HA	1:B:452:TRP:O	2.19	0.43
1:D:315:TYR:O	1:D:319:VAL:HG23	2.19	0.43
1:E:153:TYR:CZ	1:E:491:VAL:HB	2.54	0.43
1:G:300:GLN:HE22	1:G:345:VAL:HB	1.84	0.43
1:E:161:VAL:HA	1:E:188:VAL:HG23	2.01	0.43
1:B:288:GLU:OE1	1:B:325:ARG:NH2	2.52	0.42
1:A:62:ALA:O	1:A:219:ASN:ND2	2.52	0.42
1:E:461:ALA:HA	1:E:477:LEU:HD22	2.00	0.42
1:C:11:PRO:HB3	1:C:114:TYR:CE1	2.53	0.42
1:E:167:PRO:HD2	1:E:174:MET:HG3	2.01	0.42
1:G:150:PHE:CE2	1:H:458:VAL:HG21	2.54	0.42
1:B:192:LYS:HB2	1:B:232:ILE:HD11	2.01	0.42
1:G:177:TRP:NE1	1:G:477:LEU:HD21	2.35	0.42
1:G:144:ILE:HG23	1:H:462:GLN:HB3	2.02	0.42
1:B:154:THR:HA	1:B:489:LYS:O	2.19	0.42
1:C:274:PRO:HD2	1:C:428:ALA:O	2.19	0.42
1:C:241:VAL:HG23	1:C:263:LYS:HD3	2.00	0.42
1:A:167:PRO:HD2	1:A:174:MET:HG3	2.01	0.42
1:E:140:HIS:O	1:E:156:HIS:CE1	2.72	0.42
1:F:257:ALA:HB1	1:F:263:LYS:HG3	2.01	0.42
1:E:110:ASN:HB2	1:E:197:THR:HG21	2.01	0.42
1:D:225:GLY:C	1:D:227:THR:H	2.23	0.42
1:G:200:THR:O	1:G:204:VAL:HG23	2.19	0.42
1:G:331:VAL:HG12	1:G:332:GLY:N	2.35	0.42
1:H:63:VAL:HG11	1:H:235:HIS:CE1	2.54	0.42
1:B:113:PRO:HD3	1:B:298:GLN:OE1	2.20	0.42
1:H:111:GLY:O	1:H:343:PRO:HD2	2.20	0.42
1:A:271:GLY:HA2	1:A:425:TYR:HB3	2.01	0.42
1:C:302:CYS:HB3	1:C:427:LEU:CD2	2.49	0.42
1:E:70:PHE:CD1	1:E:77:ARG:HD3	2.55	0.42
1:G:70:PHE:O	1:G:70:PHE:CD2	2.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:303:CYS:SG	2:H:601:3AK:O10	2.72	0.41
1:F:109:ASP:OD2	1:F:198:PRO:HD2	2.20	0.41
1:G:33:SER:O	1:G:34:ARG:HB2	2.20	0.41
1:F:283:MET:O	1:F:287:VAL:HG23	2.20	0.41
1:C:421:ASN:O	1:C:423:SER:N	2.54	0.41
1:E:289:GLN:O	1:E:293:ALA:N	2.45	0.41
1:H:194:ALA:HB1	1:H:196:GLN:NE2	2.36	0.41
1:F:202:LEU:O	1:F:205:ALA:HB3	2.21	0.41
1:F:131:TYR:CZ	1:F:462:GLN:HA	2.55	0.41
1:A:59:VAL:O	1:A:63:VAL:HG23	2.20	0.41
1:F:500:SER:OG	1:G:77:ARG:NE	2.53	0.41
1:G:247:THR:HA	1:G:269:LEU:HD13	2.01	0.41
1:G:48:ILE:CG2	1:G:108:LEU:HD21	2.46	0.41
1:B:198:PRO:O	1:B:202:LEU:HG	2.21	0.41
1:D:361:LYS:HD3	1:D:367:LEU:HD22	2.03	0.41
1:E:78:ARG:HE	1:H:497:GLN:NE2	2.19	0.41
1:E:458:VAL:HG21	1:F:150:PHE:CE2	2.56	0.41
1:F:337:SER:O	1:F:338:LYS:HB2	2.19	0.41
1:B:381:ILE:HG22	1:B:382:GLN:O	2.21	0.41
1:D:298:GLN:HG3	1:D:341:GLN:HG3	2.02	0.41
1:A:400:ILE:O	1:A:401:PHE:CB	2.69	0.41
1:F:244:THR:HG23	1:F:268:GLU:O	2.21	0.40
1:A:153:TYR:OH	4:A:603:EDO:O1	2.34	0.40
1:F:55:ASP:HB3	1:F:58:ASP:OD2	2.21	0.40
1:H:459:PHE:HE2	1:H:465:PHE:CE2	2.39	0.40
1:G:150:PHE:CZ	1:H:458:VAL:HG21	2.57	0.40
1:G:315:TYR:CE1	1:G:319:VAL:HG21	2.56	0.40
1:H:389:VAL:HB	1:H:408:LEU:HG	2.04	0.40
1:G:102:LEU:HD21	1:G:203:TYR:CD2	2.54	0.40
1:B:240:LYS:HE3	1:B:485:TYR:CE2	2.57	0.40
1:E:99:ARG:HG3	1:E:122:LEU:HD23	2.03	0.40
1:H:149:ASP:HA	1:H:498:LYS:HB2	2.02	0.40
1:F:456:TYR:HD2	1:F:457:ASP:OD2	2.04	0.40
1:A:283:MET:O	1:A:287:VAL:HG23	2.21	0.40
1:C:205:ALA:O	1:C:208:ILE:HB	2.21	0.40
1:B:430:ALA:HB2	1:B:456:TYR:CE1	2.57	0.40
1:A:262:LEU:HD21	1:B:251:ARG:HG3	2.04	0.40
1:G:55:ASP:O	1:G:57:GLU:N	2.54	0.40
1:G:125:VAL:HG21	1:G:172:LEU:HB3	2.04	0.40
1:B:158:PRO:O	5:B:603:GAI:N3	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	492/494 (100%)	463 (94%)	29 (6%)	0	100	100
1	B	492/494 (100%)	445 (90%)	43 (9%)	4 (1%)	24	27
1	C	492/494 (100%)	457 (93%)	30 (6%)	5 (1%)	19	20
1	D	492/494 (100%)	469 (95%)	22 (4%)	1 (0%)	52	64
1	E	492/494 (100%)	468 (95%)	21 (4%)	3 (1%)	30	35
1	F	492/494 (100%)	451 (92%)	38 (8%)	3 (1%)	30	35
1	G	492/494 (100%)	456 (93%)	33 (7%)	3 (1%)	30	35
1	H	492/494 (100%)	469 (95%)	23 (5%)	0	100	100
All	All	3936/3952 (100%)	3678 (93%)	239 (6%)	19 (0%)	34	40

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	56	LYS
1	F	307	ARG
1	F	338	LYS
1	G	56	LYS
1	B	426	GLY
1	C	422	ASN
1	E	214	PRO
1	E	260	SER
1	G	383	PRO
1	D	422	ASN
1	C	56	LYS
1	F	426	GLY
1	B	41	ASN
1	B	171	PRO
1	C	11	PRO
1	C	226	PRO
1	C	371	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	198	PRO
1	E	426	GLY

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	399/399 (100%)	383 (96%)	16 (4%)	38	52
1	B	399/399 (100%)	378 (95%)	21 (5%)	28	37
1	C	399/399 (100%)	381 (96%)	18 (4%)	34	46
1	D	399/399 (100%)	389 (98%)	10 (2%)	55	72
1	E	399/399 (100%)	386 (97%)	13 (3%)	45	61
1	F	399/399 (100%)	372 (93%)	27 (7%)	20	25
1	G	399/399 (100%)	383 (96%)	16 (4%)	38	52
1	H	399/399 (100%)	387 (97%)	12 (3%)	48	65
All	All	3192/3192 (100%)	3059 (96%)	133 (4%)	36	49

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

Mol	Chain	Res	Type
1	A	41	ASN
1	A	106	GLU
1	A	117	SER
1	A	121	ASP
1	A	122	LEU
1	A	146	ILE
1	A	196	GLN
1	A	206	ASN
1	A	240	LYS
1	A	264	ARG
1	A	275	ASN
1	A	348	THR
1	A	352	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	401	PHE
1	A	462	GLN
1	A	486	THR
1	B	26	ASN
1	B	30	ASP
1	B	34	ARG
1	B	41	ASN
1	B	90	ARG
1	B	121	ASP
1	B	122	LEU
1	B	192	LYS
1	B	196	GLN
1	B	234	SER
1	B	273	SER
1	B	311	GLN
1	B	316	ASP
1	B	328	SER
1	B	359	THR
1	B	435	ASP
1	B	444	GLN
1	B	456	TYR
1	B	459	PHE
1	B	465	PHE
1	B	486	THR
1	C	20	ASN
1	C	35	LYS
1	C	41	ASN
1	C	44	THR
1	C	121	ASP
1	C	192	LYS
1	C	195	GLU
1	C	196	GLN
1	C	264	ARG
1	C	284	ASP
1	C	294	LEU
1	C	303	CYS
1	C	333	ASN
1	C	376	ASP
1	C	401	PHE
1	C	405	MET
1	C	406	GLN
1	C	437	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	41	ASN
1	D	43	SER
1	D	121	ASP
1	D	139	TYR
1	D	192	LYS
1	D	196	GLN
1	D	227	THR
1	D	275	ASN
1	D	337	SER
1	D	462	GLN
1	E	16	GLU
1	E	25	ASN
1	E	121	ASP
1	E	172	LEU
1	E	189	VAL
1	E	192	LYS
1	E	196	GLN
1	E	197	THR
1	E	275	ASN
1	E	401	PHE
1	E	462	GLN
1	E	486	THR
1	E	498	LYS
1	F	20	ASN
1	F	30	ASP
1	F	36	THR
1	F	41	ASN
1	F	49	CYS
1	F	58	ASP
1	F	112	LYS
1	F	122	LEU
1	F	159	VAL
1	F	192	LYS
1	F	196	GLN
1	F	240	LYS
1	F	260	SER
1	F	275	ASN
1	F	316	ASP
1	F	317	GLU
1	F	322	SER
1	F	327	LYS
1	F	328	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	358	ASN
1	F	376	ASP
1	F	384	THR
1	F	401	PHE
1	F	412	THR
1	F	417	VAL
1	F	427	LEU
1	F	462	GLN
1	G	14	GLN
1	G	39	THR
1	G	41	ASN
1	G	112	LYS
1	G	124	MET
1	G	135	TRP
1	G	192	LYS
1	G	196	GLN
1	G	200	THR
1	G	236	GLU
1	G	240	LYS
1	G	249	ILE
1	G	275	ASN
1	G	377	ARG
1	G	401	PHE
1	G	462	GLN
1	H	13	GLN
1	H	14	GLN
1	H	20	ASN
1	H	41	ASN
1	H	112	LYS
1	H	174	MET
1	H	192	LYS
1	H	196	GLN
1	H	275	ASN
1	H	401	PHE
1	H	463	SER
1	H	486	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	196	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	362	GLN
1	A	462	GLN
1	B	41	ASN
1	B	83	HIS
1	B	175	GLN
1	B	196	GLN
1	B	289	GLN
1	B	444	GLN
1	C	13	GLN
1	C	14	GLN
1	C	20	ASN
1	C	26	ASN
1	C	41	ASN
1	C	50	GLN
1	C	83	HIS
1	C	164	GLN
1	C	196	GLN
1	C	206	ASN
1	C	275	ASN
1	C	333	ASN
1	C	349	GLN
1	C	358	ASN
1	C	362	GLN
1	C	462	GLN
1	D	26	ASN
1	D	41	ASN
1	D	83	HIS
1	D	175	GLN
1	D	196	GLN
1	D	275	ASN
1	D	300	GLN
1	D	358	ASN
1	D	462	GLN
1	E	13	GLN
1	E	14	GLN
1	E	25	ASN
1	E	26	ASN
1	E	41	ASN
1	E	83	HIS
1	E	175	GLN
1	E	196	GLN
1	E	219	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	275	ASN
1	E	406	GLN
1	E	462	GLN
1	E	497	GLN
1	F	20	ASN
1	F	26	ASN
1	F	41	ASN
1	F	175	GLN
1	F	344	GLN
1	F	462	GLN
1	G	13	GLN
1	G	20	ASN
1	G	26	ASN
1	G	41	ASN
1	G	50	GLN
1	G	110	ASN
1	G	164	GLN
1	G	196	GLN
1	G	275	ASN
1	G	300	GLN
1	G	440	ASN
1	G	447	GLN
1	G	462	GLN
1	H	13	GLN
1	H	14	GLN
1	H	20	ASN
1	H	26	ASN
1	H	41	ASN
1	H	50	GLN
1	H	164	GLN
1	H	175	GLN
1	H	196	GLN
1	H	275	ASN
1	H	300	GLN
1	H	358	ASN
1	H	382	GLN
1	H	497	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 8 are monoatomic - leaving 19 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	$\# Z > 2$
2	3AK	A	601	-	20,20,20	2.13	4 (20%)	28,28,28	3.51	6 (21%)
4	EDO	A	603	-	3,3,3	0.33	0	2,2,2	0.72	0
4	EDO	A	604	-	3,3,3	0.36	0	2,2,2	0.44	0
5	GAI	A	605	-	0,3,3	0.00	-	0,3,3	0.00	-
2	3AK	B	601	-	20,20,20	2.04	4 (20%)	28,28,28	3.42	8 (28%)
5	GAI	B	603	-	0,3,3	0.00	-	0,3,3	0.00	-
4	EDO	C	602	-	3,3,3	0.41	0	2,2,2	0.37	0
4	EDO	C	603	-	3,3,3	0.46	0	2,2,2	0.22	0
5	GAI	C	604	-	0,3,3	0.00	-	0,3,3	0.00	-
5	GAI	D	602	-	0,3,3	0.00	-	0,3,3	0.00	-
2	3AK	E	601	-	20,20,20	2.17	4 (20%)	28,28,28	3.32	8 (28%)
4	EDO	E	603	-	3,3,3	0.38	0	2,2,2	0.42	0
4	EDO	E	604	-	3,3,3	0.40	0	2,2,2	0.37	0
4	EDO	F	602	-	3,3,3	0.39	0	2,2,2	0.41	0
5	GAI	F	603	-	0,3,3	0.00	-	0,3,3	0.00	-
5	GAI	G	602	-	0,3,3	0.00	-	0,3,3	0.00	-
2	3AK	H	601	-	20,20,20	2.08	4 (20%)	28,28,28	3.35	7 (25%)
4	EDO	H	603	-	3,3,3	0.39	0	2,2,2	0.52	0
5	GAI	H	604	-	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3AK	A	601	-	-	0/4/20/20	0/3/3/3
4	EDO	A	603	-	-	0/1/1/1	0/0/0/0
4	EDO	A	604	-	-	0/1/1/1	0/0/0/0
5	GAI	A	605	-	-	0/0/0/0	0/0/0/0
2	3AK	B	601	-	-	0/4/20/20	0/3/3/3
5	GAI	B	603	-	-	0/0/0/0	0/0/0/0
4	EDO	C	602	-	-	0/1/1/1	0/0/0/0
4	EDO	C	603	-	-	0/1/1/1	0/0/0/0
5	GAI	C	604	-	-	0/0/0/0	0/0/0/0
5	GAI	D	602	-	-	0/0/0/0	0/0/0/0
2	3AK	E	601	-	-	0/4/20/20	0/3/3/3
4	EDO	E	603	-	-	0/1/1/1	0/0/0/0
4	EDO	E	604	-	-	0/1/1/1	0/0/0/0
4	EDO	F	602	-	-	0/1/1/1	0/0/0/0
5	GAI	F	603	-	-	0/0/0/0	0/0/0/0
5	GAI	G	602	-	-	0/0/0/0	0/0/0/0
2	3AK	H	601	-	-	0/4/20/20	0/3/3/3
4	EDO	H	603	-	-	0/1/1/1	0/0/0/0
5	GAI	H	604	-	-	0/0/0/0	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	3AK	C8-C9	-4.88	1.45	1.55
2	H	601	3AK	C8-C9	-4.68	1.45	1.55
2	B	601	3AK	C8-C9	-4.66	1.45	1.55
2	E	601	3AK	C8-C9	-4.66	1.45	1.55
2	H	601	3AK	O10-C9	2.09	1.27	1.23
2	A	601	3AK	O10-C9	2.42	1.28	1.23
2	A	601	3AK	O11-C8	2.49	1.28	1.23
2	B	601	3AK	O11-C8	2.57	1.28	1.23
2	H	601	3AK	O11-C8	2.63	1.28	1.23
2	B	601	3AK	O10-C9	2.85	1.29	1.23
2	E	601	3AK	O10-C9	2.91	1.29	1.23
2	E	601	3AK	O11-C8	2.99	1.29	1.23
2	B	601	3AK	C1-C6	6.18	1.49	1.40
2	A	601	3AK	C1-C6	6.81	1.50	1.40
2	H	601	3AK	C1-C6	6.81	1.50	1.40
2	E	601	3AK	C1-C6	6.91	1.50	1.40

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	3AK	O11-C8-C9	-5.90	122.24	126.80
2	B	601	3AK	O11-C8-C9	-5.81	122.32	126.80
2	E	601	3AK	O11-C8-C9	-5.55	122.52	126.80
2	H	601	3AK	C5-C6-C1	-5.01	116.15	122.04
2	H	601	3AK	C6-C1-C9	-4.91	102.91	107.89
2	H	601	3AK	O11-C8-C9	-4.78	123.11	126.80
2	E	601	3AK	C5-C6-C1	-4.70	116.52	122.04
2	A	601	3AK	C6-C1-C9	-4.68	103.15	107.89
2	A	601	3AK	C5-C6-C1	-4.21	117.09	122.04
2	B	601	3AK	C5-C6-C1	-4.18	117.13	122.04
2	B	601	3AK	C6-C1-C9	-4.13	103.71	107.89
2	E	601	3AK	C6-C1-C9	-4.09	103.74	107.89
2	E	601	3AK	C13-C12-N7	-2.14	108.90	113.19
2	E	601	3AK	C2-C1-C6	2.24	121.75	119.20
2	H	601	3AK	C2-C1-C9	2.25	134.35	129.89
2	B	601	3AK	C2-C1-C9	2.28	134.42	129.89
2	E	601	3AK	C2-C1-C9	2.32	134.50	129.89
2	B	601	3AK	C2-C1-C6	2.34	121.87	119.20
2	A	601	3AK	C2-C1-C9	2.42	134.70	129.89
2	A	601	3AK	C2-C1-C6	2.59	122.15	119.20
2	H	601	3AK	O10-C9-C8	2.69	125.45	123.69
2	B	601	3AK	C12-N7-C8	2.89	127.88	123.63
2	E	601	3AK	O10-C9-C8	3.00	125.65	123.69
2	B	601	3AK	O10-C9-C8	3.00	125.66	123.69
2	H	601	3AK	C2-C1-C6	3.10	122.74	119.20
2	E	601	3AK	C9-C8-N7	14.19	111.80	106.02
2	H	601	3AK	C9-C8-N7	14.21	111.81	106.02
2	B	601	3AK	C9-C8-N7	14.62	111.98	106.02
2	A	601	3AK	C9-C8-N7	15.54	112.35	106.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	3AK	3	0
4	A	603	EDO	2	0
2	B	601	3AK	8	0
5	B	603	GAI	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	601	3AK	4	0
2	H	601	3AK	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 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	494/494 (100%)	0.30	24 (4%)	33 42	29, 49, 73, 111	0
1	B	494/494 (100%)	0.73	58 (11%)	6 10	29, 63, 88, 102	0
1	C	494/494 (100%)	0.36	25 (5%)	32 41	30, 52, 74, 87	0
1	D	494/494 (100%)	0.21	8 (1%)	74 80	27, 42, 63, 79	0
1	E	494/494 (100%)	0.29	19 (3%)	44 53	29, 48, 76, 106	0
1	F	494/494 (100%)	0.80	67 (13%)	4 6	26, 63, 89, 111	0
1	G	494/494 (100%)	0.37	25 (5%)	32 41	29, 54, 76, 90	0
1	H	494/494 (100%)	0.22	12 (2%)	62 71	27, 42, 65, 88	0
All	All	3952/3952 (100%)	0.41	238 (6%)	25 33	26, 50, 82, 111	0

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	345	VAL	9.1
1	F	7	ALA	8.6
1	F	255	VAL	7.8
1	F	323	VAL	7.4
1	E	247	THR	6.9
1	F	47	VAL	6.3
1	F	259	SER	6.2
1	F	318	PHE	6.1
1	C	253	ILE	5.6
1	A	258	GLY	5.4
1	A	465	PHE	5.4
1	F	250	GLY	5.3
1	F	252	VAL	5.2
1	C	247	THR	5.2
1	C	463	SER	5.2
1	G	374	ALA	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	335	PHE	5.1
1	F	374	ALA	5.1
1	B	401	PHE	4.9
1	F	39	THR	4.8
1	C	258	GLY	4.7
1	F	253	ILE	4.6
1	H	250	GLY	4.6
1	B	356	TYR	4.5
1	B	467	GLY	4.5
1	E	474	GLY	4.4
1	G	376	ASP	4.4
1	F	257	ALA	4.3
1	B	287	VAL	4.3
1	E	248	GLU	4.2
1	H	424	THR	4.2
1	F	266	THR	4.2
1	C	119	LEU	4.2
1	F	465	PHE	4.1
1	B	252	VAL	4.1
1	B	111	GLY	4.1
1	D	257	ALA	4.1
1	A	424	THR	4.1
1	C	465	PHE	4.0
1	G	106	GLU	4.0
1	F	464	PRO	3.9
1	G	32	VAL	3.9
1	F	392	GLY	3.9
1	D	471	SER	3.9
1	G	251	ARG	3.9
1	B	466	GLY	3.8
1	A	468	TYR	3.7
1	B	247	THR	3.7
1	B	255	VAL	3.7
1	A	267	LEU	3.6
1	H	465	PHE	3.6
1	G	10	ALA	3.6
1	G	477	LEU	3.5
1	F	471	SER	3.5
1	B	253	ILE	3.5
1	F	347	GLU	3.5
1	E	33	SER	3.5
1	F	53	GLU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	7	ALA	3.5
1	F	368	LEU	3.5
1	B	461	ALA	3.5
1	E	234	SER	3.5
1	B	350	PHE	3.4
1	F	44	THR	3.4
1	F	309	PHE	3.4
1	B	378	GLY	3.4
1	B	424	THR	3.4
1	A	255	VAL	3.4
1	G	255	VAL	3.4
1	D	7	ALA	3.4
1	B	465	PHE	3.4
1	F	380	PHE	3.4
1	B	463	SER	3.4
1	G	353	ILE	3.4
1	A	463	SER	3.3
1	F	246	SER	3.3
1	F	373	ILE	3.3
1	A	500	SER	3.3
1	B	340	GLU	3.3
1	C	425	TYR	3.3
1	F	32	VAL	3.3
1	F	251	ARG	3.3
1	B	386	PHE	3.2
1	F	22	ILE	3.2
1	B	362	GLN	3.2
1	C	470	MET	3.2
1	B	385	VAL	3.1
1	F	463	SER	3.1
1	F	399	GLU	3.1
1	F	170	PHE	3.1
1	E	466	GLY	3.1
1	B	381	ILE	3.0
1	F	256	ALA	3.0
1	E	467	GLY	3.0
1	B	346	ASP	3.0
1	F	23	PHE	3.0
1	B	365	ALA	3.0
1	C	377	ARG	3.0
1	A	478	GLY	3.0
1	A	256	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	247	THR	3.0
1	H	251	ARG	3.0
1	H	253	ILE	3.0
1	B	468	TYR	2.9
1	B	413	ILE	2.9
1	F	18	PHE	2.9
1	B	391	ASP	2.9
1	C	48	ILE	2.9
1	E	253	ILE	2.9
1	F	321	ARG	2.9
1	E	260	SER	2.9
1	A	22	ILE	2.9
1	G	12	ASN	2.9
1	D	399	GLU	2.8
1	B	122	LEU	2.8
1	C	114	TYR	2.8
1	E	262	LEU	2.8
1	F	108	LEU	2.8
1	F	473	SER	2.8
1	C	8	VAL	2.8
1	F	356	TYR	2.8
1	B	321	ARG	2.7
1	A	470	MET	2.7
1	A	253	ILE	2.7
1	G	104	ALA	2.7
1	H	268	GLU	2.7
1	A	466	GLY	2.7
1	F	38	PRO	2.7
1	A	473	SER	2.7
1	E	471	SER	2.7
1	H	475	ARG	2.7
1	B	367	LEU	2.6
1	B	256	ALA	2.6
1	F	379	TYR	2.6
1	F	395	ILE	2.6
1	E	266	THR	2.6
1	E	465	PHE	2.6
1	H	248	GLU	2.6
1	F	351	LYS	2.6
1	D	266	THR	2.6
1	C	254	GLN	2.6
1	F	243	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	472	GLY	2.6
1	F	345	VAL	2.6
1	B	470	MET	2.6
1	G	465	PHE	2.5
1	F	15	PRO	2.5
1	C	255	VAL	2.5
1	F	477	LEU	2.5
1	F	378	GLY	2.5
1	G	37	PHE	2.5
1	G	473	SER	2.5
1	E	265	VAL	2.5
1	F	50	GLN	2.5
1	B	474	GLY	2.5
1	C	197	THR	2.5
1	H	246	SER	2.5
1	D	268	GLU	2.5
1	D	500	SER	2.5
1	A	254	GLN	2.5
1	G	356	TYR	2.5
1	C	481	GLY	2.4
1	B	25	ASN	2.4
1	C	464	PRO	2.4
1	F	199	LEU	2.4
1	F	329	ARG	2.4
1	B	265	VAL	2.4
1	E	229	GLY	2.4
1	B	473	SER	2.4
1	C	259	SER	2.4
1	F	334	PRO	2.4
1	A	356	TYR	2.4
1	B	318	PHE	2.4
1	F	350	PHE	2.4
1	G	350	PHE	2.4
1	C	257	ALA	2.4
1	B	250	GLY	2.4
1	G	17	VAL	2.4
1	B	243	PHE	2.4
1	F	173	LEU	2.3
1	B	197	THR	2.3
1	H	271	GLY	2.3
1	A	480	TYR	2.3
1	A	464	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	384	THR	2.3
1	B	226	PRO	2.3
1	B	409	LYS	2.3
1	H	423	SER	2.3
1	F	301	CYS	2.3
1	B	388	ASP	2.3
1	B	469	LYS	2.3
1	C	249	ILE	2.3
1	B	347	GLU	2.3
1	A	223	GLY	2.3
1	G	399	GLU	2.3
1	B	270	GLY	2.2
1	F	245	GLY	2.2
1	B	376	ASP	2.2
1	B	251	ARG	2.2
1	C	250	GLY	2.2
1	F	265	VAL	2.2
1	F	363	GLU	2.2
1	D	477	LEU	2.2
1	F	348	THR	2.2
1	B	7	ALA	2.2
1	G	27	GLU	2.2
1	E	224	PHE	2.2
1	B	358	ASN	2.2
1	G	16	GLU	2.2
1	B	369	CYS	2.2
1	G	471	SER	2.2
1	B	257	ALA	2.1
1	F	106	GLU	2.1
1	C	458	VAL	2.1
1	C	224	PHE	2.1
1	B	105	LEU	2.1
1	B	262	LEU	2.1
1	A	247	THR	2.1
1	B	10	ALA	2.1
1	G	201	ALA	2.1
1	G	463	SER	2.1
1	E	122	LEU	2.1
1	G	14	GLN	2.1
1	F	432	PHE	2.1
1	F	474	GLY	2.1
1	F	48	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	105	LEU	2.1
1	C	467	GLY	2.1
1	B	325	ARG	2.1
1	A	251	ARG	2.0
1	G	254	GLN	2.0
1	E	269	LEU	2.0
1	F	52	ALA	2.0
1	F	470	MET	2.0
1	E	475	ARG	2.0
1	B	232	ILE	2.0
1	B	13	GLN	2.0
1	F	194	ALA	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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	EDO	H	603	4/4	0.92	0.36	16.13	71,71,72,73	0
4	EDO	C	603	4/4	0.87	0.45	13.98	60,65,67,68	0
4	EDO	C	602	4/4	0.90	0.31	11.99	63,64,64,65	0
4	EDO	A	604	4/4	0.92	0.32	9.90	65,67,67,69	0
4	EDO	E	603	4/4	0.94	0.35	7.94	81,86,88,89	0
5	GAI	F	603	4/4	0.89	0.33	5.67	73,74,74,75	0
4	EDO	E	604	4/4	0.87	0.26	4.54	75,78,78,80	0
3	NA	A	602	1/1	0.82	0.22	3.99	91,91,91,91	0
3	NA	C	601	1/1	0.65	0.27	2.35	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GAI	H	604	4/4	0.95	0.16	2.07	70,75,75,77	0
5	GAI	B	603	4/4	0.78	0.27	1.97	93,93,94,95	0
3	NA	B	602	1/1	0.81	0.30	1.82	93,93,93,93	0
2	3AK	E	601	18/18	0.91	0.20	1.62	43,46,49,50	0
3	NA	E	602	1/1	0.77	0.17	1.53	73,73,73,73	0
5	GAI	G	602	4/4	0.97	0.15	1.37	66,66,69,71	0
4	EDO	A	603	4/4	0.91	0.17	1.30	68,71,72,75	0
4	EDO	F	602	4/4	0.83	0.17	1.16	80,82,82,83	0
3	NA	G	601	1/1	0.74	0.21	1.12	83,83,83,83	0
2	3AK	B	601	18/18	0.84	0.22	1.05	46,51,56,57	0
3	NA	D	601	1/1	0.75	0.15	0.64	64,64,64,64	0
5	GAI	C	604	4/4	0.93	0.16	0.63	74,75,75,75	0
2	3AK	A	601	18/18	0.90	0.20	0.56	42,50,59,59	0
2	3AK	H	601	18/18	0.92	0.18	0.30	47,54,63,64	0
5	GAI	A	605	4/4	0.95	0.18	0.26	69,72,73,76	0
5	GAI	D	602	4/4	0.83	0.15	-0.11	74,77,79,79	0
3	NA	F	601	1/1	0.83	0.17	-0.64	84,84,84,84	0
3	NA	H	602	1/1	0.88	0.11	-2.49	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.