



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:46 am GMT

PDB ID : 1AA1
Title : ACTIVATED SPINACH RUBISCO IN COMPLEX WITH THE PRODUCT
3-PHOSPHOGLYCERATE
Authors : Taylor, T.C.; Andersson, I.
Deposited on : 1997-01-20
Resolution : 2.20 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

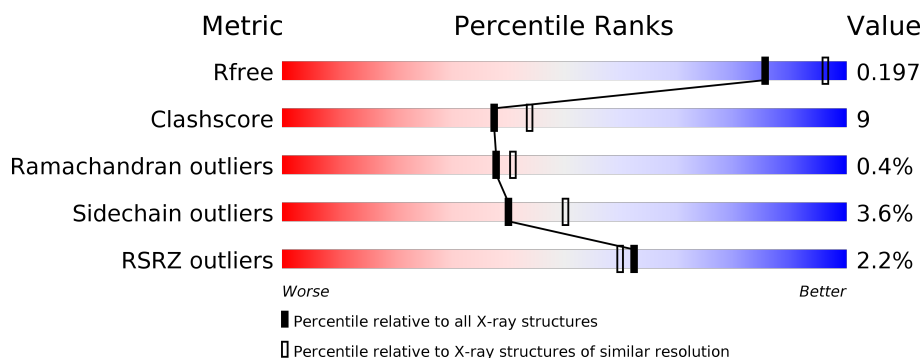
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



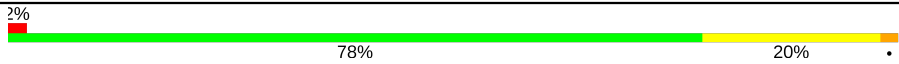

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	B	475	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>8%</div> </div> </div>
1	E	475	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>8%</div> </div> </div>
1	H	475	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>8%</div> </div> </div>
1	L	475	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>8%</div> </div> </div>
2	C	123	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>19%</div> <div>.</div> </div> </div>
2	F	123	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>.</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	123	
2	S	123	

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
4	3PG	B	478	-	-	-	X
4	3PG	E	478	-	-	-	X
4	3PG	H	478	-	-	-	X
4	3PG	L	478	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 18956 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 RIBULOSE BISPHOSPHATE CARBOXYLASE (LARGE CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	438	Total	C	N	O	S	0	0	0
			3431	2172	607	635	17			
1	B	438	Total	C	N	O	S	0	0	0
			3431	2172	607	635	17			
1	E	438	Total	C	N	O	S	0	0	0
			3431	2172	607	635	17			
1	H	438	Total	C	N	O	S	0	0	0
			3431	2172	607	635	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	201	KCX	LYS	MODIFIED RESIDUE	UNP P00875
B	201	KCX	LYS	MODIFIED RESIDUE	UNP P00875
E	201	KCX	LYS	MODIFIED RESIDUE	UNP P00875
H	201	KCX	LYS	MODIFIED RESIDUE	UNP P00875

- Molecule 2 is a protein called RIBULOSE BISPHOSPHATE CARBOXYLASE (SMALL CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	123	Total	C	N	O	S	0	0	0
			1033	673	167	186	7			
2	C	123	Total	C	N	O	S	0	0	0
			1033	673	167	186	7			
2	F	123	Total	C	N	O	S	0	0	0
			1033	673	167	186	7			
2	I	123	Total	C	N	O	S	0	0	0
			1033	673	167	186	7			

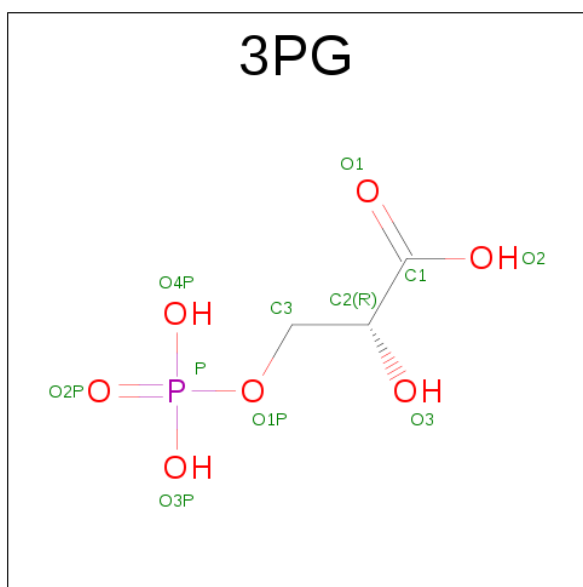
There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	2	GLN	LYS	CONFLICT	UNP Q43832
S	6	ILE	THR	CONFLICT	UNP Q43832
S	7	LEU	GLN	CONFLICT	UNP Q43832
S	9	LEU	MET	CONFLICT	UNP Q43832
S	11	LYS	ARG	CONFLICT	UNP Q43832
S	109	GLU	GLN	CONFLICT	UNP Q43832
S	113	ILE	VAL	CONFLICT	UNP Q43832
C	2	GLN	LYS	CONFLICT	UNP Q43832
C	6	ILE	THR	CONFLICT	UNP Q43832
C	7	LEU	GLN	CONFLICT	UNP Q43832
C	9	LEU	MET	CONFLICT	UNP Q43832
C	11	LYS	ARG	CONFLICT	UNP Q43832
C	109	GLU	GLN	CONFLICT	UNP Q43832
C	113	ILE	VAL	CONFLICT	UNP Q43832
F	2	GLN	LYS	CONFLICT	UNP Q43832
F	6	ILE	THR	CONFLICT	UNP Q43832
F	7	LEU	GLN	CONFLICT	UNP Q43832
F	9	LEU	MET	CONFLICT	UNP Q43832
F	11	LYS	ARG	CONFLICT	UNP Q43832
F	109	GLU	GLN	CONFLICT	UNP Q43832
F	113	ILE	VAL	CONFLICT	UNP Q43832
I	2	GLN	LYS	CONFLICT	UNP Q43832
I	6	ILE	THR	CONFLICT	UNP Q43832
I	7	LEU	GLN	CONFLICT	UNP Q43832
I	9	LEU	MET	CONFLICT	UNP Q43832
I	11	LYS	ARG	CONFLICT	UNP Q43832
I	109	GLU	GLN	CONFLICT	UNP Q43832
I	113	ILE	VAL	CONFLICT	UNP Q43832

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	L	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0

- Molecule 4 is 3-PHOSPHOGLYCERIC ACID (three-letter code: 3PG) (formula: C₃H₇O₇P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	L	1	Total	C	O	P	0	0
			11	3	7	1		
4	L	1	Total	C	O	P	0	0
			11	3	7	1		
4	B	1	Total	C	O	P	0	0
			11	3	7	1		
4	B	1	Total	C	O	P	0	0
			11	3	7	1		
4	E	1	Total	C	O	P	0	0
			11	3	7	1		
4	E	1	Total	C	O	P	0	0
			11	3	7	1		
4	H	1	Total	C	O	P	0	0
			11	3	7	1		
4	H	1	Total	C	O	P	0	0
			11	3	7	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	202	Total	O	0	0
			202	202		
5	C	52	Total	O	0	0
			52	52		
5	E	201	Total	O	0	0
			201	201		
5	F	52	Total	O	0	0
			52	52		

Continued on next page...

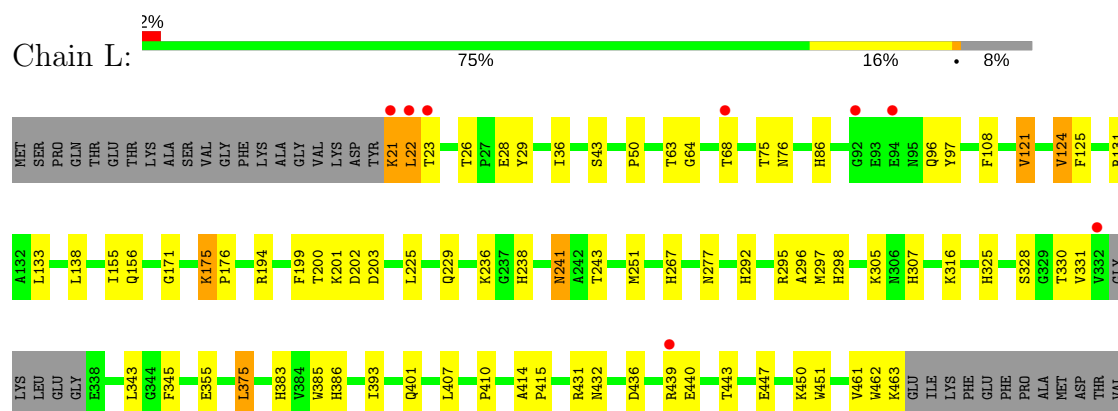
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	199	Total 199	O 199	0	0
5	I	52	Total 52	O 52	0	0
5	L	201	Total 201	O 201	0	0
5	S	49	Total 49	O 49	0	0

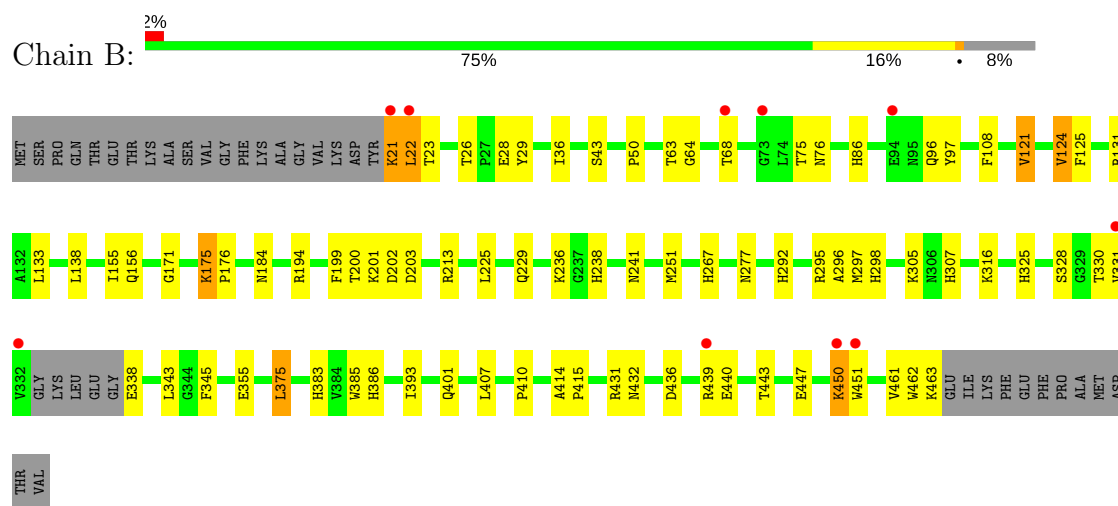
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

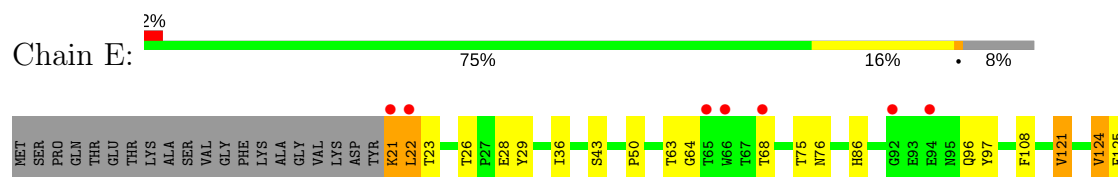
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE (LARGE CHAIN)

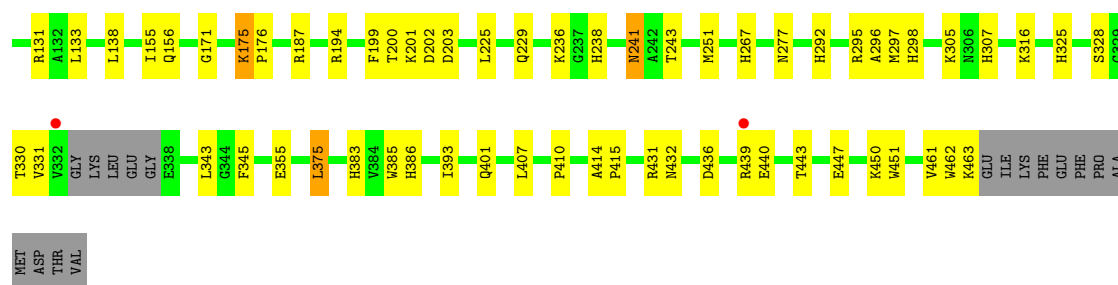


• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE (LARGE CHAIN)

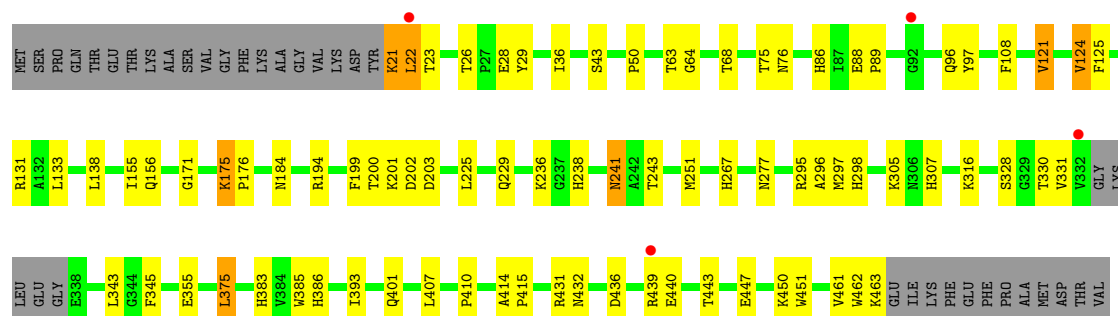
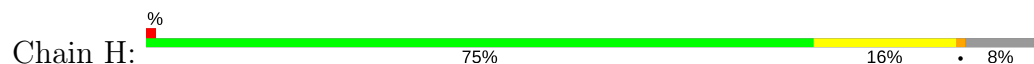


• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE (LARGE CHAIN)

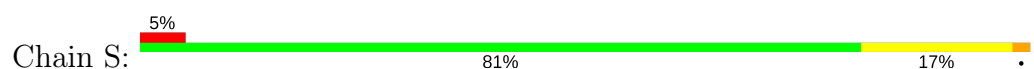




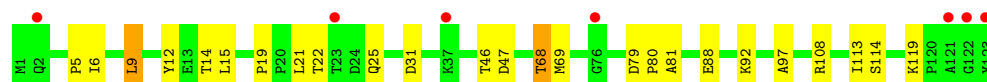
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE (LARGE CHAIN)



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE (SMALL CHAIN)



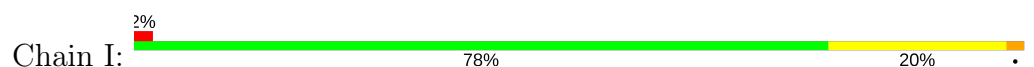
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE (SMALL CHAIN)

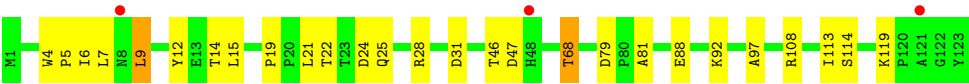


• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE (SMALL CHAIN)



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE (SMALL CHAIN)





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	157.60Å 158.70Å 203.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20 19.90 – 2.20	Depositor EDS
% Data completeness (in resolution range)	83.8 (7.00-2.20) 84.6 (19.90-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.25 (at 2.21Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.207 , 0.224 0.199 , 0.197	Depositor DCC
R_{free} test set	3147 reflections (3.02%)	DCC
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 72.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18956	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.69 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.6882e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, KCX, 3PG

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	B	0.41	0/3502	0.68	1/4753 (0.0%)
1	E	0.41	0/3502	0.68	1/4753 (0.0%)
1	H	0.41	0/3502	0.68	1/4753 (0.0%)
1	L	0.41	0/3502	0.68	1/4753 (0.0%)
2	C	0.42	0/1068	0.64	0/1453
2	F	0.42	0/1068	0.64	0/1453
2	I	0.42	0/1068	0.64	0/1453
2	S	0.42	0/1068	0.64	0/1453
All	All	0.41	0/18280	0.67	4/24824 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	462	TRP	N-CA-C	5.58	126.06	111.00
1	L	462	TRP	N-CA-C	5.56	126.02	111.00
1	E	462	TRP	N-CA-C	5.56	126.01	111.00
1	H	462	TRP	N-CA-C	5.56	126.01	111.00

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	B	3431	0	3343	62	6
1	E	3431	0	3343	60	0
1	H	3431	0	3343	61	2
1	L	3431	0	3343	59	2
2	C	1033	0	990	23	0
2	F	1033	0	990	23	0
2	I	1033	0	990	25	2
2	S	1033	0	990	22	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	H	1	0	0	0	0
3	L	1	0	0	0	0
4	B	22	0	8	6	0
4	E	22	0	8	6	0
4	H	22	0	8	6	0
4	L	22	0	8	6	0
5	B	202	0	0	6	6
5	C	52	0	0	4	0
5	E	201	0	0	4	4
5	F	52	0	0	4	0
5	H	199	0	0	5	3
5	I	52	0	0	4	0
5	L	201	0	0	4	2
5	S	49	0	0	4	0
All	All	18956	0	17364	310	15

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 9.

All (310) 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)
2:S:68:THR:HG21	2:C:6:ILE:HG12	1.56	0.87
1:B:267:HIS:HD2	1:B:277:ASN:HD22	1.26	0.83
1:H:267:HIS:HD2	1:H:277:ASN:HD22	1.26	0.83
1:L:267:HIS:HD2	1:L:277:ASN:HD22	1.26	0.83
1:E:267:HIS:HD2	1:E:277:ASN:HD22	1.26	0.82
1:E:175:LYS:NZ	4:E:477:3PG:H2	1.99	0.78
1:B:175:LYS:NZ	4:B:477:3PG:H2	1.99	0.78
1:H:175:LYS:NZ	4:H:477:3PG:H2	1.99	0.78
2:S:6:ILE:HG12	2:I:68:THR:HG21	1.63	0.77
1:L:175:LYS:NZ	4:L:477:3PG:H2	1.99	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:385:TRP:NE1	1:H:463:LYS:HB2	2.00	0.77
2:F:68:THR:HG21	2:I:6:ILE:HG12	1.65	0.77
1:L:385:TRP:NE1	1:L:463:LYS:HB2	2.00	0.76
1:E:385:TRP:NE1	1:E:463:LYS:HB2	2.00	0.76
1:B:298:HIS:CE1	4:B:478:3PG:H31	2.22	0.75
1:H:298:HIS:CE1	4:H:478:3PG:H31	2.22	0.75
1:B:385:TRP:NE1	1:B:463:LYS:HB2	2.00	0.74
1:E:298:HIS:CE1	4:E:478:3PG:H31	2.22	0.74
1:L:175:LYS:HZ1	4:L:477:3PG:H2	1.50	0.74
1:L:298:HIS:CE1	4:L:478:3PG:H31	2.22	0.74
5:F:708:HOH:O	2:I:6:ILE:HG21	1.88	0.73
2:S:6:ILE:HG21	5:I:164:HOH:O	1.90	0.70
1:H:75:THR:HG22	1:H:76:ASN:H	1.56	0.69
2:C:68:THR:HG21	2:F:6:ILE:HG12	1.73	0.69
1:L:75:THR:HG22	1:L:76:ASN:H	1.57	0.69
1:E:75:THR:HG22	1:E:76:ASN:H	1.57	0.69
5:S:157:HOH:O	2:C:6:ILE:HG21	1.92	0.68
1:B:75:THR:HG22	1:B:76:ASN:H	1.56	0.68
1:B:229:GLN:HE21	1:B:236:LYS:H	1.44	0.66
1:H:383:HIS:H	1:H:386:HIS:HD2	1.44	0.66
1:L:229:GLN:HE21	1:L:236:LYS:H	1.44	0.66
1:E:383:HIS:H	1:E:386:HIS:HD2	1.44	0.65
5:C:456:HOH:O	2:F:6:ILE:HG21	1.96	0.65
1:E:229:GLN:HE21	1:E:236:LYS:H	1.44	0.65
1:L:383:HIS:H	1:L:386:HIS:HD2	1.44	0.65
1:E:414:ALA:HB3	1:E:415:PRO:HD3	1.79	0.64
1:H:229:GLN:HE21	1:H:236:LYS:H	1.44	0.64
1:B:383:HIS:H	1:B:386:HIS:HD2	1.44	0.64
1:H:414:ALA:HB3	1:H:415:PRO:HD3	1.79	0.64
1:L:414:ALA:HB3	1:L:415:PRO:HD3	1.79	0.63
1:B:414:ALA:HB3	1:B:415:PRO:HD3	1.79	0.63
1:H:298:HIS:NE2	4:H:478:3PG:H31	2.13	0.63
1:L:298:HIS:NE2	4:L:478:3PG:H31	2.13	0.63
1:E:298:HIS:NE2	4:E:478:3PG:H31	2.13	0.63
1:H:175:LYS:HZ2	4:H:477:3PG:H2	1.64	0.62
1:B:298:HIS:NE2	4:B:478:3PG:H31	2.13	0.62
1:E:175:LYS:HZ2	4:E:477:3PG:H2	1.64	0.62
1:L:171:GLY:HA3	1:L:401:GLN:NE2	2.15	0.61
1:H:21:LYS:HD2	1:H:22:LEU:N	2.15	0.61
1:B:171:GLY:HA3	1:B:401:GLN:NE2	2.15	0.61
1:E:21:LYS:HD2	1:E:22:LEU:N	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LYS:HZ2	4:B:477:3PG:H2	1.64	0.61
1:L:21:LYS:HD2	1:L:22:LEU:N	2.15	0.61
1:E:171:GLY:HA3	1:E:401:GLN:NE2	2.16	0.60
1:B:21:LYS:HD2	1:B:22:LEU:N	2.15	0.60
1:H:121:VAL:HG22	1:H:125:PHE:CE1	2.36	0.60
1:B:121:VAL:HG22	1:B:125:PHE:CE1	2.36	0.60
1:H:171:GLY:HA3	1:H:401:GLN:NE2	2.16	0.60
1:E:121:VAL:HG22	1:E:125:PHE:CE1	2.36	0.60
1:E:175:LYS:HZ1	4:E:477:3PG:H2	1.66	0.60
1:H:443:THR:O	1:H:447:GLU:HG3	2.02	0.60
1:E:443:THR:O	1:E:447:GLU:HG3	2.02	0.60
1:B:175:LYS:HZ1	4:B:477:3PG:H2	1.66	0.59
1:L:443:THR:O	1:L:447:GLU:HG3	2.02	0.59
1:B:443:THR:O	1:B:447:GLU:HG3	2.02	0.59
1:H:175:LYS:HZ1	4:H:477:3PG:H2	1.66	0.59
1:L:121:VAL:HG22	1:L:125:PHE:CE1	2.36	0.59
2:F:5:PRO:HB2	2:F:9:LEU:HG	1.85	0.58
1:L:436:ASP:O	1:L:440:GLU:HG2	2.03	0.58
1:E:436:ASP:O	1:E:440:GLU:HG2	2.03	0.58
1:H:436:ASP:O	1:H:440:GLU:HG2	2.03	0.58
1:L:331:VAL:HG11	1:L:393:ILE:HD13	1.86	0.58
1:B:436:ASP:O	1:B:440:GLU:HG2	2.03	0.58
2:C:5:PRO:HB2	2:C:9:LEU:HG	1.85	0.58
1:B:50:PRO:HG3	1:B:97:TYR:CZ	2.39	0.57
1:H:50:PRO:HG3	1:H:97:TYR:CZ	2.39	0.57
1:B:331:VAL:HG11	1:B:393:ILE:HD13	1.85	0.57
2:S:5:PRO:HB2	2:S:9:LEU:HG	1.85	0.57
1:E:331:VAL:HG11	1:E:393:ILE:HD13	1.86	0.57
1:L:50:PRO:HG3	1:L:97:TYR:CZ	2.39	0.57
1:L:75:THR:HG22	1:L:76:ASN:N	2.19	0.57
1:B:75:THR:HG22	1:B:76:ASN:N	2.19	0.57
1:H:331:VAL:HG11	1:H:393:ILE:HD13	1.85	0.57
1:B:267:HIS:CD2	1:B:277:ASN:HD22	2.16	0.57
1:E:50:PRO:HG3	1:E:97:TYR:CZ	2.39	0.57
2:I:5:PRO:HB2	2:I:9:LEU:HG	1.85	0.57
1:B:68:THR:HA	5:B:611:HOH:O	2.05	0.57
1:E:75:THR:HG22	1:E:76:ASN:N	2.19	0.56
1:L:68:THR:HA	5:L:603:HOH:O	2.05	0.56
1:E:68:THR:HA	5:E:611:HOH:O	2.05	0.56
1:H:75:THR:HG22	1:H:76:ASN:N	2.19	0.56
2:S:12:TYR:CE1	2:S:119:LYS:HD3	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:TYR:CE1	2:C:119:LYS:HD3	2.41	0.56
2:I:12:TYR:CE1	2:I:119:LYS:HD3	2.41	0.56
1:H:68:THR:HA	5:H:614:HOH:O	2.05	0.56
1:B:410:PRO:HD3	1:B:461:VAL:HG21	1.87	0.56
2:F:12:TYR:CE1	2:F:119:LYS:HD3	2.41	0.56
1:H:410:PRO:HD3	1:H:461:VAL:HG21	1.87	0.55
1:L:267:HIS:CD2	1:L:277:ASN:HD22	2.16	0.55
1:L:26:THR:HG22	1:L:29:TYR:HB2	1.89	0.55
1:E:431:ARG:HH21	1:E:432:ASN:HD21	1.55	0.55
1:E:410:PRO:HD3	1:E:461:VAL:HG21	1.87	0.55
1:H:431:ARG:HH21	1:H:432:ASN:HD21	1.55	0.55
1:L:410:PRO:HD3	1:L:461:VAL:HG21	1.87	0.55
1:B:36:ILE:HD13	1:B:108:PHE:CE1	2.42	0.55
1:E:26:THR:HG22	1:E:29:TYR:HB2	1.89	0.55
1:H:36:ILE:HD13	1:H:108:PHE:CE1	2.42	0.55
1:L:36:ILE:HD13	1:L:108:PHE:CE1	2.42	0.54
1:B:431:ARG:HH21	1:B:432:ASN:HD21	1.55	0.54
1:E:36:ILE:HD13	1:E:108:PHE:CE1	2.42	0.54
2:S:108:ARG:HD2	5:S:150:HOH:O	2.08	0.54
1:E:200:THR:OG1	1:E:238:HIS:HD2	1.91	0.54
1:H:26:THR:HG22	1:H:29:TYR:HB2	1.89	0.54
2:C:108:ARG:HD2	5:C:417:HOH:O	2.08	0.54
1:B:201:KCX:OQ2	1:B:203:ASP:HA	2.08	0.54
1:H:200:THR:OG1	1:H:238:HIS:HD2	1.91	0.54
1:B:86:HIS:HE1	5:B:657:HOH:O	1.91	0.54
1:L:201:KCX:OQ2	1:L:203:ASP:HA	2.08	0.54
1:B:200:THR:OG1	1:B:238:HIS:HD2	1.91	0.54
1:L:431:ARG:HH21	1:L:432:ASN:HD21	1.55	0.54
1:E:201:KCX:OQ2	1:E:203:ASP:HA	2.08	0.53
1:H:156:GLN:HE21	2:I:108:ARG:NH2	2.06	0.53
1:B:26:THR:HG22	1:B:29:TYR:HB2	1.89	0.53
1:H:201:KCX:OQ2	1:H:203:ASP:HA	2.08	0.53
1:E:156:GLN:HE21	2:F:108:ARG:NH2	2.07	0.53
1:B:156:GLN:HE21	2:C:108:ARG:NH2	2.07	0.53
1:E:267:HIS:CD2	1:E:277:ASN:HD22	2.16	0.53
1:E:86:HIS:HE1	5:E:656:HOH:O	1.91	0.53
1:L:200:THR:OG1	1:L:238:HIS:HD2	1.91	0.53
2:I:22:THR:OG1	2:I:25:GLN:HG2	2.09	0.53
1:B:124:VAL:HG22	5:B:591:HOH:O	2.09	0.53
1:E:124:VAL:HG22	5:E:591:HOH:O	2.09	0.53
2:F:22:THR:OG1	2:F:25:GLN:HG2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:108:ARG:HD2	5:F:669:HOH:O	2.07	0.52
1:L:124:VAL:HG22	5:L:583:HOH:O	2.09	0.52
1:E:155:ILE:HG12	1:E:375:LEU:HD13	1.91	0.52
2:C:22:THR:OG1	2:C:25:GLN:HG2	2.09	0.52
2:S:22:THR:OG1	2:S:25:GLN:HG2	2.09	0.52
1:H:86:HIS:HE1	5:H:659:HOH:O	1.91	0.52
2:I:108:ARG:HD2	5:I:156:HOH:O	2.08	0.52
1:L:156:GLN:HE21	2:S:108:ARG:NH2	2.07	0.52
1:H:155:ILE:HG12	1:H:375:LEU:HD13	1.91	0.52
1:B:155:ILE:HG12	1:B:375:LEU:HD13	1.92	0.52
1:H:124:VAL:HG22	5:H:594:HOH:O	2.09	0.52
1:L:86:HIS:HE1	5:L:648:HOH:O	1.91	0.52
2:F:79:ASP:OD2	2:F:81:ALA:HB3	2.11	0.51
1:L:155:ILE:HG12	1:L:375:LEU:HD13	1.91	0.51
2:C:79:ASP:OD2	2:C:81:ALA:HB3	2.11	0.51
2:S:79:ASP:OD2	2:S:81:ALA:HB3	2.11	0.51
1:E:26:THR:CG2	1:E:29:TYR:HB2	2.41	0.50
1:B:26:THR:CG2	1:B:29:TYR:HB2	2.41	0.50
1:L:171:GLY:HA3	1:L:401:GLN:HE21	1.77	0.50
1:H:267:HIS:CD2	1:H:277:ASN:HD22	2.16	0.50
1:H:86:HIS:CE1	5:H:659:HOH:O	2.65	0.49
1:L:202:ASP:OD1	1:L:238:HIS:HE1	1.95	0.49
1:H:26:THR:CG2	1:H:29:TYR:HB2	2.41	0.49
1:L:26:THR:CG2	1:L:29:TYR:HB2	2.41	0.49
1:E:297:MET:O	1:E:297:MET:HG2	2.13	0.49
1:H:202:ASP:OD1	1:H:238:HIS:HE1	1.95	0.49
1:L:86:HIS:CE1	5:L:648:HOH:O	2.65	0.49
1:E:175:LYS:HA	1:E:176:PRO:C	2.33	0.49
1:E:86:HIS:CE1	5:E:656:HOH:O	2.65	0.49
1:E:96:GLN:HE22	1:E:305:LYS:NZ	2.11	0.49
2:I:79:ASP:OD2	2:I:81:ALA:HB3	2.11	0.49
1:L:175:LYS:HA	1:L:176:PRO:C	2.33	0.49
1:L:96:GLN:HE22	1:L:305:LYS:NZ	2.11	0.49
1:H:175:LYS:HA	1:H:176:PRO:C	2.33	0.49
1:B:96:GLN:HE22	1:B:305:LYS:NZ	2.11	0.49
1:H:171:GLY:HA3	1:H:401:GLN:HE21	1.77	0.48
1:B:175:LYS:HA	1:B:176:PRO:C	2.33	0.48
1:E:202:ASP:OD1	1:E:238:HIS:HE1	1.95	0.48
1:L:297:MET:O	1:L:297:MET:HG2	2.13	0.48
1:H:96:GLN:HE22	1:H:305:LYS:NZ	2.11	0.48
1:B:202:ASP:OD1	1:B:238:HIS:HE1	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:MET:O	1:B:297:MET:HG2	2.13	0.48
1:B:171:GLY:HA3	1:B:401:GLN:HE21	1.77	0.48
1:B:343:LEU:HD21	1:B:393:ILE:HG23	1.95	0.48
2:F:46:THR:HG22	2:F:97:ALA:HB2	1.95	0.48
1:H:343:LEU:HD21	1:H:393:ILE:HG23	1.95	0.48
2:I:46:THR:HG22	2:I:97:ALA:HB2	1.96	0.48
1:E:343:LEU:HD21	1:E:393:ILE:HG23	1.95	0.48
1:H:297:MET:HG2	1:H:297:MET:O	2.13	0.48
1:B:86:HIS:CE1	5:B:657:HOH:O	2.65	0.47
1:E:171:GLY:HA3	1:E:401:GLN:HE21	1.77	0.47
1:B:138:LEU:O	1:B:316:LYS:NZ	2.46	0.47
2:C:46:THR:HG22	2:C:97:ALA:HB2	1.95	0.47
1:E:138:LEU:O	1:E:316:LYS:NZ	2.46	0.47
2:F:14:THR:HG22	2:F:15:LEU:HG	1.97	0.47
2:S:46:THR:HG22	2:S:97:ALA:HB2	1.95	0.47
1:L:343:LEU:HD21	1:L:393:ILE:HG23	1.95	0.47
1:H:26:THR:HG23	1:H:28:GLU:OE2	2.15	0.47
1:E:26:THR:HG23	1:E:28:GLU:OE2	2.15	0.47
1:L:26:THR:HG23	1:L:28:GLU:OE2	2.15	0.47
1:B:26:THR:HG23	1:B:28:GLU:OE2	2.15	0.46
2:I:14:THR:HG22	2:I:15:LEU:HG	1.97	0.46
1:B:383:HIS:CE1	1:B:385:TRP:HB2	2.51	0.46
1:E:383:HIS:CE1	1:E:385:TRP:HB2	2.51	0.46
1:H:156:GLN:HE21	2:I:108:ARG:CZ	2.29	0.46
2:C:14:THR:HG22	2:C:15:LEU:HG	1.97	0.46
1:L:156:GLN:HE21	2:S:108:ARG:CZ	2.29	0.46
1:H:383:HIS:CE1	1:H:385:TRP:HB2	2.51	0.45
2:S:14:THR:HG22	2:S:15:LEU:HG	1.97	0.45
1:L:175:LYS:HZ2	4:L:477:3PG:H2	1.80	0.45
1:E:156:GLN:HE21	2:F:108:ARG:CZ	2.29	0.45
1:H:138:LEU:O	1:H:316:LYS:NZ	2.46	0.45
1:L:383:HIS:CE1	1:L:385:TRP:HB2	2.51	0.45
1:B:156:GLN:HE21	2:C:108:ARG:CZ	2.29	0.45
2:C:21:LEU:HA	2:C:25:GLN:HE21	1.82	0.45
2:I:21:LEU:HA	2:I:25:GLN:HE21	1.82	0.45
1:H:328:SER:HB2	1:H:345:PHE:HE1	1.82	0.45
2:I:108:ARG:HB2	5:I:156:HOH:O	2.17	0.45
1:L:328:SER:HB2	1:L:345:PHE:HE1	1.82	0.45
2:S:21:LEU:HA	2:S:25:GLN:HE21	1.82	0.45
1:E:328:SER:HB2	1:E:345:PHE:HE1	1.82	0.44
2:F:21:LEU:HA	2:F:25:GLN:HE21	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:431:ARG:HE	1:L:432:ASN:ND2	2.16	0.44
2:S:68:THR:HG21	2:C:6:ILE:CG1	2.39	0.44
2:S:108:ARG:HB2	5:S:150:HOH:O	2.17	0.44
1:B:296:ALA:O	1:B:297:MET:HB3	2.18	0.44
1:E:431:ARG:HE	1:E:432:ASN:ND2	2.16	0.44
1:B:431:ARG:HE	1:B:432:ASN:ND2	2.16	0.44
1:H:171:GLY:HA2	1:H:199:PHE:O	2.18	0.44
1:B:328:SER:HB2	1:B:345:PHE:HE1	1.82	0.43
1:E:171:GLY:HA2	1:E:199:PHE:O	2.18	0.43
1:E:296:ALA:O	1:E:297:MET:HB3	2.18	0.43
1:L:138:LEU:O	1:L:316:LYS:NZ	2.46	0.43
1:B:194:ARG:NH1	2:C:6:ILE:HD12	2.34	0.43
1:H:431:ARG:HE	1:H:432:ASN:ND2	2.16	0.43
1:L:194:ARG:NH1	2:S:6:ILE:HD12	2.34	0.43
1:L:296:ALA:O	1:L:297:MET:HB3	2.18	0.43
1:B:330:THR:O	1:B:331:VAL:HB	2.19	0.43
1:H:296:ALA:O	1:H:297:MET:HB3	2.18	0.43
1:L:171:GLY:HA2	1:L:199:PHE:O	2.18	0.43
1:E:295:ARG:HH21	4:E:478:3PG:H32	1.84	0.43
2:F:108:ARG:HB2	5:F:669:HOH:O	2.17	0.43
1:L:463:LYS:HD2	1:L:463:LYS:HA	1.83	0.43
1:B:295:ARG:HH21	4:B:478:3PG:H32	1.84	0.43
2:C:22:THR:H	2:C:25:GLN:CG	2.32	0.43
1:H:295:ARG:HH21	4:H:478:3PG:H32	1.84	0.43
1:B:251:MET:HE2	1:B:251:MET:HB3	1.83	0.43
2:C:79:ASP:HA	2:C:80:PRO:HD3	1.93	0.43
1:L:133:LEU:O	1:L:307:HIS:HA	2.19	0.43
1:B:133:LEU:O	1:B:307:HIS:HA	2.19	0.43
1:E:330:THR:O	1:E:331:VAL:HB	2.19	0.43
2:F:22:THR:H	2:F:25:GLN:CG	2.32	0.43
1:H:330:THR:O	1:H:331:VAL:HB	2.19	0.43
2:S:22:THR:H	2:S:25:GLN:CG	2.32	0.43
2:C:108:ARG:HB2	5:C:417:HOH:O	2.17	0.42
1:H:133:LEU:O	1:H:307:HIS:HA	2.19	0.42
1:L:330:THR:O	1:L:331:VAL:HB	2.19	0.42
1:E:43:SER:HB3	1:E:131:ARG:CZ	2.50	0.42
1:E:194:ARG:NH1	2:F:6:ILE:HD12	2.34	0.42
1:B:43:SER:HB3	1:B:131:ARG:CZ	2.50	0.42
2:F:25:GLN:HB2	5:F:724:HOH:O	2.20	0.42
2:C:46:THR:CG2	2:C:97:ALA:HB2	2.50	0.42
2:I:22:THR:H	2:I:25:GLN:CG	2.32	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:43:SER:HB3	1:L:131:ARG:CZ	2.50	0.42
1:L:295:ARG:HH21	4:L:478:3PG:H32	1.84	0.42
1:B:171:GLY:HA2	1:B:199:PHE:O	2.18	0.42
2:F:46:THR:CG2	2:F:97:ALA:HB2	2.50	0.42
1:E:133:LEU:O	1:E:307:HIS:HA	2.19	0.42
2:F:68:THR:HG21	2:I:6:ILE:CG1	2.41	0.42
2:I:25:GLN:HB2	5:I:169:HOH:O	2.20	0.42
2:S:46:THR:CG2	2:S:97:ALA:HB2	2.50	0.42
1:B:436:ASP:OD2	1:B:439:ARG:HG3	2.20	0.42
1:B:463:LYS:HD2	1:B:463:LYS:HA	1.83	0.42
2:C:69:MET:CE	1:E:187:ARG:HD3	2.50	0.42
1:H:251:MET:HE2	1:H:251:MET:HB3	1.86	0.42
1:L:251:MET:HE2	1:L:251:MET:HB3	1.87	0.42
1:H:194:ARG:NH1	2:I:6:ILE:HD12	2.34	0.41
1:E:436:ASP:OD2	1:E:439:ARG:HG3	2.20	0.41
1:E:451:TRP:CH2	2:F:19:PRO:HD3	2.55	0.41
1:H:121:VAL:HG22	1:H:125:PHE:HE1	1.85	0.41
1:H:43:SER:HB3	1:H:131:ARG:CZ	2.50	0.41
1:B:451:TRP:CH2	2:C:19:PRO:HD3	2.55	0.41
2:C:25:GLN:HB2	5:C:472:HOH:O	2.20	0.41
1:B:213:ARG:HA	1:B:213:ARG:HD3	1.85	0.41
2:F:9:LEU:HD22	2:F:9:LEU:HA	1.90	0.41
2:I:46:THR:CG2	2:I:97:ALA:HB2	2.50	0.41
1:B:175:LYS:HE2	1:B:175:LYS:HB3	1.84	0.41
1:L:436:ASP:OD2	1:L:439:ARG:HG3	2.20	0.41
1:H:451:TRP:CH2	2:I:19:PRO:HD3	2.55	0.41
2:I:9:LEU:HA	2:I:9:LEU:HD22	1.90	0.41
1:E:251:MET:HB3	1:E:251:MET:HE2	1.88	0.41
2:F:113:ILE:HG22	2:F:114:SER:N	2.35	0.41
2:F:96:ASN:HD21	2:I:7:LEU:HD11	1.86	0.41
2:S:113:ILE:HG22	2:S:114:SER:N	2.35	0.41
1:L:451:TRP:CH2	2:S:19:PRO:HD3	2.55	0.41
1:B:338:GLU:N	5:B:673:HOH:O	2.54	0.41
1:H:436:ASP:OD2	1:H:439:ARG:HG3	2.21	0.41
1:B:175:LYS:HG3	1:B:407:LEU:HD12	2.03	0.41
1:B:184:ASN:ND2	5:B:519:HOH:O	2.54	0.41
2:C:113:ILE:HG22	2:C:114:SER:N	2.35	0.41
1:E:241:ASN:ND2	1:E:243:THR:H	2.19	0.41
2:S:25:GLN:HB2	5:S:162:HOH:O	2.20	0.41
1:E:175:LYS:HG3	1:E:407:LEU:HD12	2.03	0.41
1:H:88:GLU:HA	1:H:89:PRO:HD3	1.95	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:GLN:NE2	1:E:236:LYS:H	2.16	0.41
1:L:292:HIS:HA	1:L:325:HIS:HB2	2.03	0.41
1:L:241:ASN:ND2	1:L:243:THR:H	2.19	0.40
1:L:175:LYS:HG3	1:L:407:LEU:HD12	2.03	0.40
1:B:292:HIS:HA	1:B:325:HIS:HB2	2.03	0.40
1:E:292:HIS:HA	1:E:325:HIS:HB2	2.03	0.40
1:H:175:LYS:HG3	1:H:407:LEU:HD12	2.03	0.40
1:H:241:ASN:ND2	1:H:243:THR:H	2.19	0.40
2:I:113:ILE:HG22	2:I:114:SER:N	2.35	0.40
2:I:4:TRP:HA	2:I:5:PRO:HD3	1.89	0.40
1:H:184:ASN:ND2	5:H:522:HOH:O	2.54	0.40
1:H:175:LYS:HB3	1:H:175:LYS:HE2	1.84	0.40
2:S:6:ILE:CG1	2:I:68:THR:HG21	2.42	0.40

All (15) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:650:HOH:O	5:E:657:HOH:O[8_455]	0.83	1.37
1:H:451:TRP:O	5:H:661:HOH:O[4_555]	0.92	1.28
5:B:657:HOH:O	5:E:656:HOH:O[7_555]	1.12	1.08
1:L:451:TRP:CD1	5:E:658:HOH:O[8_455]	1.19	1.01
5:L:648:HOH:O	5:H:659:HOH:O[7_455]	1.31	0.89
1:H:451:TRP:C	5:H:661:HOH:O[4_555]	1.61	0.59
1:B:450:LYS:CG	5:B:659:HOH:O[4_565]	1.62	0.58
1:L:451:TRP:NE1	5:E:658:HOH:O[8_455]	1.88	0.32
2:I:24:ASP:OD2	2:I:28:ARG:NH2[4_555]	1.95	0.25
1:B:450:LYS:NZ	5:B:659:HOH:O[4_565]	2.01	0.19
1:B:450:LYS:N	5:B:659:HOH:O[4_565]	2.03	0.17
1:B:450:LYS:CA	5:B:659:HOH:O[4_565]	2.07	0.13
1:B:450:LYS:O	1:B:450:LYS:CE[4_565]	2.11	0.09
1:B:450:LYS:CB	5:B:659:HOH:O[4_565]	2.13	0.07
2:I:24:ASP:OD2	2:I:28:ARG:NE[4_555]	2.16	0.04

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	B	433/475 (91%)	416 (96%)	15 (4%)	2 (0%)	32	34
1	E	433/475 (91%)	416 (96%)	15 (4%)	2 (0%)	32	34
1	H	433/475 (91%)	416 (96%)	15 (4%)	2 (0%)	32	34
1	L	433/475 (91%)	416 (96%)	15 (4%)	2 (0%)	32	34
2	C	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
2	F	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
2	I	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
2	S	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
All	All	2216/2392 (93%)	2128 (96%)	80 (4%)	8 (0%)	38	41

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	63	THR
1	L	64	GLY
1	B	63	THR
1	B	64	GLY
1	E	63	THR
1	E	64	GLY
1	H	63	THR
1	H	64	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	B	355/385 (92%)	344 (97%)	11 (3%)	45	57
1	E	355/385 (92%)	344 (97%)	11 (3%)	45	57
1	H	355/385 (92%)	344 (97%)	11 (3%)	45	57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	355/385 (92%)	344 (97%)	11 (3%)	45	57
2	C	112/112 (100%)	106 (95%)	6 (5%)	26	30
2	F	112/112 (100%)	106 (95%)	6 (5%)	26	30
2	I	112/112 (100%)	106 (95%)	6 (5%)	26	30
2	S	112/112 (100%)	106 (95%)	6 (5%)	26	30
All	All	1868/1988 (94%)	1800 (96%)	68 (4%)	40	50

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LYS
1	L	22	LEU
1	L	23	THR
1	L	121	VAL
1	L	124	VAL
1	L	175	LYS
1	L	225	LEU
1	L	241	ASN
1	L	355	GLU
1	L	375	LEU
1	L	450	LYS
2	S	9	LEU
2	S	31	ASP
2	S	47	ASP
2	S	68	THR
2	S	88	GLU
2	S	92	LYS
1	B	21	LYS
1	B	22	LEU
1	B	23	THR
1	B	121	VAL
1	B	124	VAL
1	B	175	LYS
1	B	225	LEU
1	B	241	ASN
1	B	355	GLU
1	B	375	LEU
1	B	450	LYS
2	C	9	LEU
2	C	31	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	47	ASP
2	C	68	THR
2	C	88	GLU
2	C	92	LYS
1	E	21	LYS
1	E	22	LEU
1	E	23	THR
1	E	121	VAL
1	E	124	VAL
1	E	175	LYS
1	E	225	LEU
1	E	241	ASN
1	E	355	GLU
1	E	375	LEU
1	E	450	LYS
2	F	9	LEU
2	F	31	ASP
2	F	47	ASP
2	F	68	THR
2	F	88	GLU
2	F	92	LYS
1	H	21	LYS
1	H	22	LEU
1	H	23	THR
1	H	121	VAL
1	H	124	VAL
1	H	175	LYS
1	H	225	LEU
1	H	241	ASN
1	H	355	GLU
1	H	375	LEU
1	H	450	LYS
2	I	9	LEU
2	I	31	ASP
2	I	47	ASP
2	I	68	THR
2	I	88	GLU
2	I	92	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	96	GLN
1	L	153	HIS
1	L	156	GLN
1	L	163	ASN
1	L	184	ASN
1	L	207	ASN
1	L	229	GLN
1	L	238	HIS
1	L	241	ASN
1	L	267	HIS
1	L	277	ASN
1	L	282	HIS
1	L	304	GLN
1	L	386	HIS
1	L	401	GLN
1	L	420	ASN
1	L	432	ASN
2	S	25	GLN
2	S	29	GLN
1	B	96	GLN
1	B	153	HIS
1	B	156	GLN
1	B	163	ASN
1	B	184	ASN
1	B	207	ASN
1	B	229	GLN
1	B	238	HIS
1	B	241	ASN
1	B	267	HIS
1	B	277	ASN
1	B	282	HIS
1	B	304	GLN
1	B	386	HIS
1	B	401	GLN
1	B	432	ASN
2	C	25	GLN
2	C	29	GLN
1	E	96	GLN
1	E	153	HIS
1	E	156	GLN
1	E	163	ASN
1	E	184	ASN
1	E	207	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	229	GLN
1	E	238	HIS
1	E	241	ASN
1	E	267	HIS
1	E	277	ASN
1	E	282	HIS
1	E	304	GLN
1	E	386	HIS
1	E	420	ASN
1	E	432	ASN
2	F	25	GLN
2	F	29	GLN
1	H	96	GLN
1	H	153	HIS
1	H	156	GLN
1	H	163	ASN
1	H	184	ASN
1	H	207	ASN
1	H	229	GLN
1	H	238	HIS
1	H	241	ASN
1	H	267	HIS
1	H	277	ASN
1	H	282	HIS
1	H	304	GLN
1	H	386	HIS
1	H	401	GLN
1	H	432	ASN
2	I	25	GLN
2	I	29	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	KCX	B	201	1,3	8,11,12	0.64	0	6,12,14	1.22	0
1	KCX	E	201	1,3	8,11,12	0.65	0	6,12,14	1.23	0
1	KCX	H	201	1,3	8,11,12	0.64	0	6,12,14	1.23	0
1	KCX	L	201	1,3	8,11,12	0.65	0	6,12,14	1.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	B	201	1,3	-	0/6/10/12	0/0/0/0
1	KCX	E	201	1,3	-	0/6/10/12	0/0/0/0
1	KCX	H	201	1,3	-	0/6/10/12	0/0/0/0
1	KCX	L	201	1,3	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	201	KCX	1	0
1	E	201	KCX	1	0
1	H	201	KCX	1	0
1	L	201	KCX	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
4	3PG	B	477	3	7,10,10	2.03	2 (28%)	10,14,14	1.67	3 (30%)
4	3PG	B	478	-	7,10,10	1.21	1 (14%)	10,14,14	3.78	4 (40%)
4	3PG	E	477	3	7,10,10	2.04	2 (28%)	10,14,14	1.66	3 (30%)
4	3PG	E	478	-	7,10,10	1.20	1 (14%)	10,14,14	3.78	4 (40%)
4	3PG	H	477	3	7,10,10	2.04	2 (28%)	10,14,14	1.66	3 (30%)
4	3PG	H	478	-	7,10,10	1.21	1 (14%)	10,14,14	3.78	4 (40%)
4	3PG	L	477	3	7,10,10	2.03	2 (28%)	10,14,14	1.66	3 (30%)
4	3PG	L	478	-	7,10,10	1.21	1 (14%)	10,14,14	3.78	4 (40%)

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
4	3PG	B	477	3	-	0/6/10/10	0/0/0/0
4	3PG	B	478	-	-	0/6/10/10	0/0/0/0
4	3PG	E	477	3	-	0/6/10/10	0/0/0/0
4	3PG	E	478	-	-	0/6/10/10	0/0/0/0
4	3PG	H	477	3	-	0/6/10/10	0/0/0/0
4	3PG	H	478	-	-	0/6/10/10	0/0/0/0
4	3PG	L	477	3	-	0/6/10/10	0/0/0/0
4	3PG	L	478	-	-	0/6/10/10	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	478	3PG	P-O1P	2.74	1.69	1.60
4	H	478	3PG	P-O1P	2.76	1.69	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	478	3PG	P-O1P	2.76	1.69	1.60
4	B	478	3PG	P-O1P	2.77	1.69	1.60
4	H	477	3PG	P-O1P	2.92	1.69	1.60
4	L	477	3PG	P-O1P	2.94	1.69	1.60
4	B	477	3PG	P-O1P	2.94	1.69	1.60
4	E	477	3PG	P-O1P	2.95	1.69	1.60
4	L	477	3PG	C3-C2	3.73	1.64	1.50
4	H	477	3PG	C3-C2	3.73	1.64	1.50
4	E	477	3PG	C3-C2	3.74	1.64	1.50
4	B	477	3PG	C3-C2	3.75	1.64	1.50

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	478	3PG	O3-C2-C3	-3.42	99.19	110.43
4	H	478	3PG	O3-C2-C3	-3.42	99.20	110.43
4	L	478	3PG	O3-C2-C3	-3.42	99.21	110.43
4	B	478	3PG	O3-C2-C3	-3.41	99.23	110.43
4	L	478	3PG	P-O1P-C3	-3.27	109.28	118.30
4	E	478	3PG	P-O1P-C3	-3.27	109.29	118.30
4	B	478	3PG	P-O1P-C3	-3.27	109.29	118.30
4	H	478	3PG	P-O1P-C3	-3.26	109.32	118.30
4	H	478	3PG	O1P-P-O2P	-2.99	98.08	106.47
4	L	478	3PG	O1P-P-O2P	-2.98	98.11	106.47
4	B	478	3PG	O1P-P-O2P	-2.98	98.12	106.47
4	E	478	3PG	O1P-P-O2P	-2.97	98.15	106.47
4	B	477	3PG	O4P-P-O1P	-2.75	99.42	106.73
4	L	477	3PG	O4P-P-O1P	-2.74	99.45	106.73
4	E	477	3PG	O4P-P-O1P	-2.73	99.46	106.73
4	H	477	3PG	O4P-P-O1P	-2.72	99.50	106.73
4	E	477	3PG	O3P-P-O1P	-2.19	100.90	106.73
4	B	477	3PG	O3P-P-O1P	-2.18	100.92	106.73
4	L	477	3PG	O3P-P-O1P	-2.18	100.93	106.73
4	H	477	3PG	O3P-P-O1P	-2.17	100.95	106.73
4	B	477	3PG	O4P-P-O3P	2.06	115.94	107.61
4	L	477	3PG	O4P-P-O3P	2.07	115.96	107.61
4	H	477	3PG	O4P-P-O3P	2.07	115.98	107.61
4	E	477	3PG	O4P-P-O3P	2.08	115.99	107.61
4	L	478	3PG	O1P-C3-C2	10.00	136.81	107.94
4	H	478	3PG	O1P-C3-C2	10.00	136.81	107.94
4	B	478	3PG	O1P-C3-C2	10.01	136.82	107.94
4	E	478	3PG	O1P-C3-C2	10.01	136.84	107.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	477	3PG	3	0
4	B	478	3PG	3	0
4	E	477	3PG	3	0
4	E	478	3PG	3	0
4	H	477	3PG	3	0
4	H	478	3PG	3	0
4	L	477	3PG	3	0
4	L	478	3PG	3	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	B	437/475 (92%)	-0.36	10 (2%) 61 58	4, 13, 36, 50	0
1	E	437/475 (92%)	-0.49	9 (2%) 64 61	4, 13, 36, 50	0
1	H	437/475 (92%)	-0.54	4 (0%) 84 83	4, 13, 36, 50	0
1	L	437/475 (92%)	-0.51	8 (1%) 69 66	4, 13, 36, 50	0
2	C	123/123 (100%)	0.11	7 (5%) 24 24	9, 26, 40, 47	0
2	F	123/123 (100%)	-0.04	3 (2%) 59 57	9, 26, 40, 47	0
2	I	123/123 (100%)	-0.08	3 (2%) 59 57	9, 26, 40, 47	0
2	S	123/123 (100%)	0.18	6 (4%) 30 29	9, 26, 40, 47	0
All	All	2240/2392 (93%)	-0.36	50 (2%) 62 60	4, 17, 39, 50	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	LEU	5.6
1	H	22	LEU	5.5
2	I	121	ALA	5.4
1	B	332	VAL	5.2
2	F	121	ALA	4.9
1	L	22	LEU	4.6
1	E	92	GLY	4.6
2	S	122	GLY	4.4
1	B	439	ARG	4.0
1	E	21	LYS	3.9
1	H	332	VAL	3.9
2	C	121	ALA	3.7
1	L	94	GLU	3.6
1	E	22	LEU	3.6
1	E	439	ARG	3.6
1	L	332	VAL	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	21	LYS	3.3
2	S	121	ALA	3.2
2	F	122	GLY	3.0
1	B	451	TRP	2.9
1	B	331	VAL	2.9
1	B	450	LYS	2.8
1	B	68	THR	2.8
2	S	108	ARG	2.8
1	E	94	GLU	2.7
2	C	122	GLY	2.7
1	H	439	ARG	2.6
2	S	92	LYS	2.6
1	E	332	VAL	2.6
1	L	439	ARG	2.6
1	B	21	LYS	2.5
2	F	92	LYS	2.5
2	C	2	GLN	2.5
1	B	94	GLU	2.5
2	C	23	THR	2.3
2	C	76	GLY	2.3
2	S	123	TYR	2.3
2	I	48	HIS	2.3
2	I	8	ASN	2.3
2	C	37	LYS	2.3
1	H	92	GLY	2.2
1	E	65	THR	2.2
1	E	66	TRP	2.2
1	B	73	GLY	2.1
2	S	107	ASN	2.1
2	C	123	TYR	2.1
1	L	68	THR	2.0
1	E	68	THR	2.0
1	L	92	GLY	2.0
1	L	23	THR	2.0

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

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(\AA^2)	Q<0.9
1	KCX	E	201	12/13	0.92	0.12	-	6,17,29,35	0
1	KCX	H	201	12/13	0.96	0.12	-	6,17,29,35	0
1	KCX	B	201	12/13	0.91	0.13	-	6,17,29,35	0
1	KCX	L	201	12/13	0.94	0.12	-	6,17,29,35	0

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(\AA^2)	Q<0.9
4	3PG	H	478	11/11	0.89	0.22	3.75	41,44,47,49	0
4	3PG	B	478	11/11	0.88	0.25	3.35	41,44,47,49	0
4	3PG	E	478	11/11	0.86	0.23	3.25	41,44,47,49	0
4	3PG	L	478	11/11	0.92	0.19	3.10	41,44,47,49	0
4	3PG	E	477	11/11	0.89	0.19	1.00	35,38,43,46	0
4	3PG	L	477	11/11	0.91	0.17	0.75	35,38,43,46	0
4	3PG	H	477	11/11	0.94	0.16	0.59	35,38,43,46	0
4	3PG	B	477	11/11	0.91	0.15	0.20	35,38,43,46	0
3	MG	H	476	1/1	0.82	0.08	-	29,29,29,29	0
3	MG	L	476	1/1	0.88	0.13	-	29,29,29,29	0
3	MG	E	476	1/1	0.65	0.18	-	29,29,29,29	0
3	MG	B	476	1/1	0.86	0.11	-	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.