



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:20 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 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/ValidationPDFNotes.html>

---

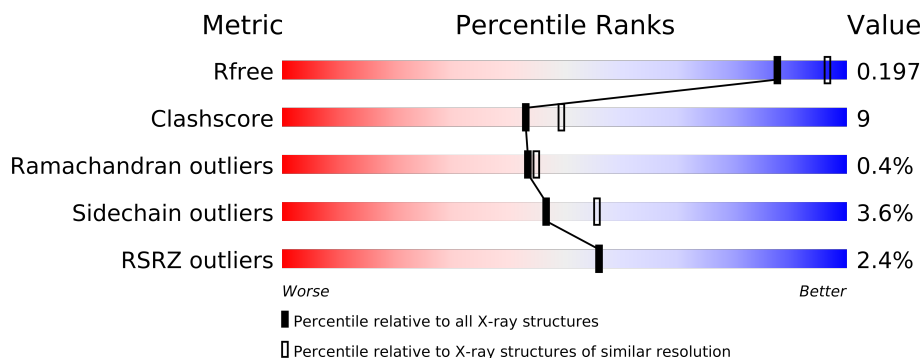
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	475	
1	E	475	
1	H	475	
1	L	475	
2	C	123	
2	F	123	
2	I	123	
2	S	123	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	E	476	-	X

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	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

There are 5 unique types of molecules in this entry. The entry contains 18956 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

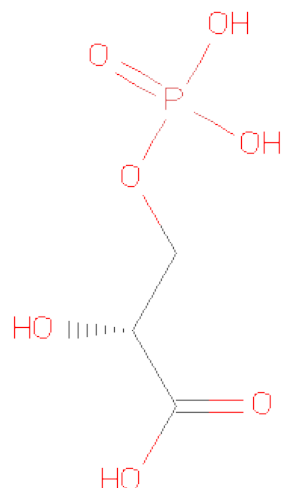
There are 28 discrepancies between the modelled and reference sequences:

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: C<sub>3</sub>H<sub>7</sub>O<sub>7</sub>P).



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...*

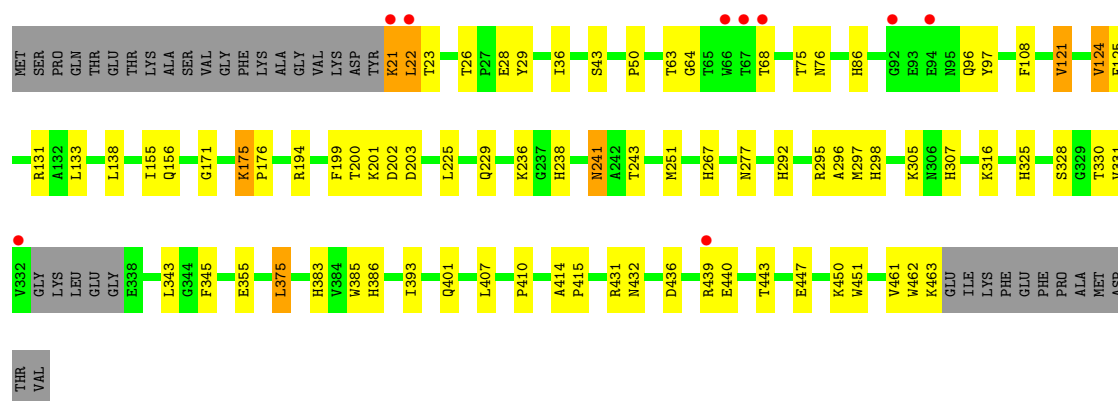
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	199	Total 199	O 199	0	0
5	I	52	Total 52	O 52	0	0
5	L	201	Total 201	O 201	0	0
5	S	49	Total 49	O 49	0	0

### 3 Residue-property plots

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.

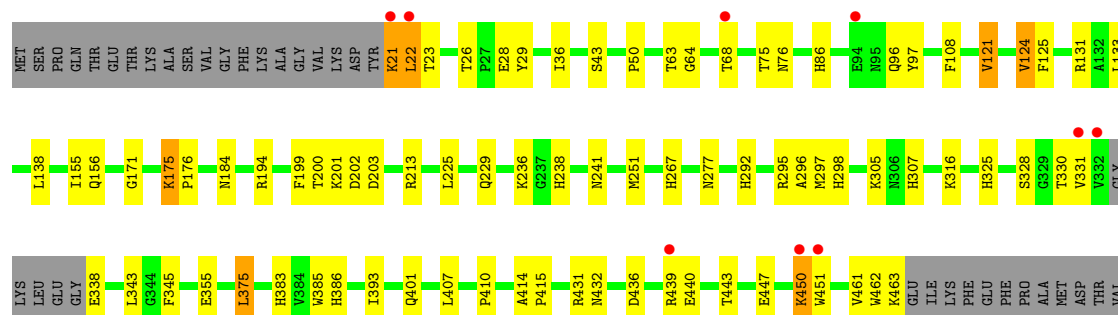
#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE (LARGE CHAIN)

Chain L: 



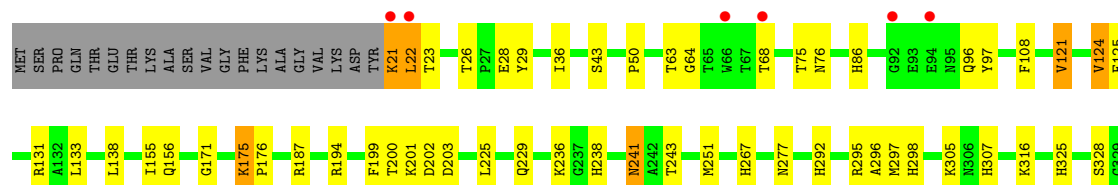
#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE (LARGE CHAIN)

Chain B: 

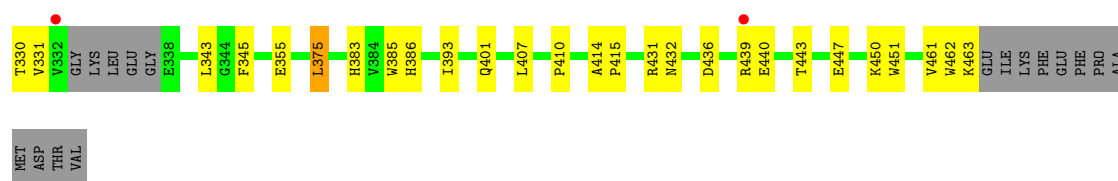


#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE (LARGE CHAIN)

Chain E: 

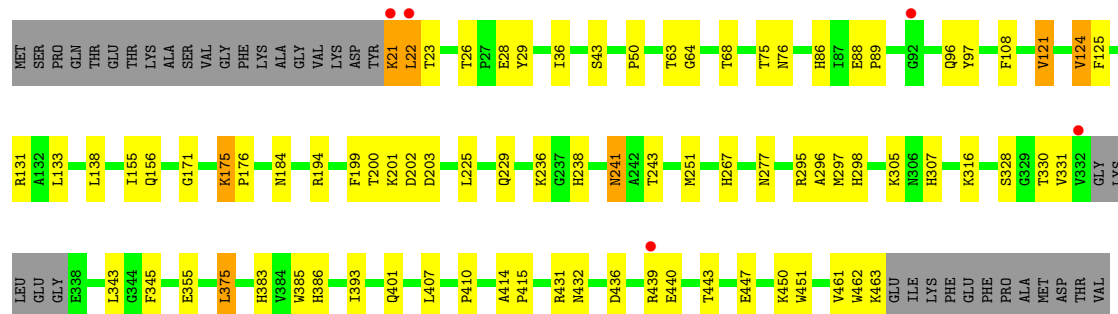






- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE (LARGE CHAIN)

Chain H:



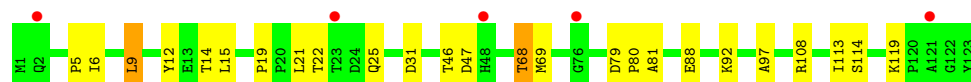
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE (SMALL CHAIN)

Chain S:



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE (SMALL CHAIN)

Chain C:



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE (SMALL CHAIN)

Chain F:



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE (SMALL CHAIN)

Chain I:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 84.5 (19.90-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.25 (at 2.21Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.207 , 0.224 0.200 , 0.197	Depositor DCC
$R_{free}$ test set	3147 reflections (3.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 58.9	EDS
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 107959 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

## 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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	7
5	C	52	0	0	4	0
5	E	201	0	0	4	8
5	F	52	0	0	4	0
5	H	199	0	0	5	4
5	I	52	0	0	4	0
5	L	201	0	0	4	6
5	S	49	0	0	4	0
All	All	18956	0	17364	310	20

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (310) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:175:LYS:NZ	4:L:477:3PG:H2	1.99	0.77
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:L:175:LYS:HZ1	4:L:477:3PG:H2	1.50	0.74
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: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:E:21:LYS:HD2	1:E:22:LEU:N	2.15	0.61
1:B:171:GLY:HA3	1:B:401:GLN:NE2	2.15	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(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:H:171:GLY:HA3	1:H:401:GLN:NE2	2.16	0.60
1:B:121:VAL:HG22	1:B: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:121:VAL:HG22	1:E:125:PHE:CE1	2.36	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:H:175:LYS:HZ1	4:H:477:3PG:H2	1.66	0.59
1:B:443:THR:O	1:B:447:GLU:HG3	2.02	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:H:436:ASP:O	1:H:440:GLU:HG2	2.03	0.58
1:E:436:ASP:O	1:E:440:GLU:HG2	2.03	0.58
1:L:331:VAL:HG11	1:L:393:ILE:HD13	1.86	0.58
2:C:5:PRO:HB2	2:C:9:LEU:HG	1.85	0.58
1:B:436:ASP:O	1:B:440:GLU:HG2	2.03	0.58
1:H:50:PRO:HG3	1:H:97:TYR:CZ	2.39	0.57
1:B:50:PRO:HG3	1:B:97:TYR:CZ	2.39	0.57
2:S:5:PRO:HB2	2:S:9:LEU:HG	1.85	0.57
1:B:331:VAL:HG11	1:B:393:ILE:HD13	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
2:I:5:PRO:HB2	2:I:9:LEU:HG	1.85	0.57
1:E:50:PRO:HG3	1:E:97:TYR:CZ	2.39	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
2:C:12:TYR:CE1	2:C:119:LYS:HD3	2.41	0.56

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:L:156:GLN:HE21	2:S:108:ARG:NH2	2.07	0.52
2:I:108:ARG:HD2	5:I:156:HOH:O	2.08	0.52
1:H:86:HIS:HE1	5:H:659:HOH:O	1.91	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:L:86:HIS:HE1	5:L:648:HOH:O	1.91	0.52
1:H:124:VAL:HG22	5:H:594:HOH:O	2.09	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:L:202:ASP:OD1	1:L:238:HIS:HE1	1.95	0.49
1:H:86:HIS:CE1	5:H:659:HOH:O	2.65	0.49
1:L:26:THR:CG2	1:L:29:TYR:HB2	2.41	0.49
1:H:26:THR:CG2	1:H:29:TYR:HB2	2.41	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:297:MET:O	1:E:297:MET:HG2	2.13	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
1:L:175:LYS:HA	1:L:176:PRO:C	2.33	0.49
2:I:79:ASP:OD2	2:I:81:ALA:HB3	2.11	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
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

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:343:LEU:HD21	1:H:393:ILE:HG23	1.95	0.48
2:F:46:THR:HG22	2:F:97:ALA:HB2	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:E:171:GLY:HA3	1:E:401:GLN:HE21	1.77	0.47
1:B:86:HIS:CE1	5:B:657:HOH:O	2.65	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:S:46:THR:HG22	2:S:97:ALA:HB2	1.95	0.47
2:F:14:THR:HG22	2:F:15:LEU:HG	1.97	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:E:383:HIS:CE1	1:E:385:TRP:HB2	2.51	0.46
1:B:383:HIS:CE1	1:B: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:L:383:HIS:CE1	1:L:385:TRP:HB2	2.51	0.45
1:H:138:LEU:O	1:H:316:LYS:NZ	2.46	0.45
1:B:156:GLN:HE21	2:C:108:ARG:CZ	2.29	0.45
2:I:21:LEU:HA	2:I:25:GLN:HE21	1.82	0.45
2:C:21:LEU:HA	2:C:25:GLN:HE21	1.82	0.45
2:I:108:ARG:HB2	5:I:156:HOH:O	2.17	0.45
1:H:328:SER:HB2	1:H:345:PHE:HE1	1.82	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
2:S:68:THR:HG21	2:C:6:ILE:CG1	2.39	0.44
1:L:431:ARG:HE	1:L:432:ASN:ND2	2.16	0.44
2:F:21:LEU:HA	2:F:25:GLN:HE21	1.82	0.44
1:E:328:SER:HB2	1:E:345:PHE:HE1	1.82	0.44
2:S:108:ARG:HB2	5:S:150:HOH:O	2.17	0.44
1:E:431:ARG:HE	1:E:432:ASN:ND2	2.16	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:296:ALA:O	1:B:297:MET:HB3	2.18	0.44
1:H:171:GLY:HA2	1:H:199:PHE:O	2.18	0.44
1:B:431:ARG:HE	1:B:432:ASN:ND2	2.16	0.44
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:B:328:SER:HB2	1:B:345:PHE:HE1	1.82	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:L:194:ARG:NH1	2:S:6:ILE:HD12	2.34	0.43
1:H:431:ARG:HE	1:H:432:ASN:ND2	2.16	0.43
1:L:296:ALA:O	1:L:297:MET:HB3	2.18	0.43
1:L:171:GLY:HA2	1:L:199:PHE:O	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:463:LYS:HD2	1:L:463:LYS:HA	1.83	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:B:295:ARG:HH21	4:B:478:3PG:H32	1.84	0.43
1:H:295:ARG:HH21	4:H:478:3PG:H32	1.84	0.43
2:C:22:THR:H	2:C:25:GLN:CG	2.32	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:251:MET:HE2	1:B:251:MET:HB3	1.83	0.43
1:E:330:THR:O	1:E:331:VAL:HB	2.19	0.43
1:H:330:THR:O	1:H:331:VAL:HB	2.19	0.43
2:F:22:THR:H	2:F:25:GLN:CG	2.32	0.43
2:S:22:THR:H	2:S:25:GLN:CG	2.32	0.43
1:B:133:LEU:O	1:B:307:HIS:HA	2.19	0.43
1:L:330:THR:O	1:L:331:VAL:HB	2.19	0.42
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:E:194:ARG:NH1	2:F:6:ILE:HD12	2.34	0.42
1:E:43:SER:HB3	1:E:131:ARG:CZ	2.50	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
1:L:295:ARG:HH21	4:L:478:3PG:H32	1.84	0.42
2:I:22:THR:H	2:I:25:GLN:CG	2.32	0.42
2:C:46:THR:CG2	2:C:97:ALA:HB2	2.50	0.42
1:L:43:SER:HB3	1:L:131:ARG:CZ	2.50	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
2:F:68:THR:HG21	2:I:6:ILE:CG1	2.41	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:E:133:LEU:O	1:E:307:HIS:HA	2.19	0.42
1:B:463:LYS:HD2	1:B:463:LYS:HA	1.83	0.42
1:B:436:ASP:OD2	1:B:439:ARG:HG3	2.20	0.42
1:L:251:MET:HE2	1:L:251:MET:HB3	1.87	0.42
1:H:251:MET:HE2	1:H:251:MET:HB3	1.86	0.42
2:C:69:MET:CE	1:E:187:ARG:HD3	2.50	0.42
1:H:194:ARG:NH1	2:I:6:ILE:HD12	2.34	0.41
1:H:121:VAL:HG22	1:H:125:PHE:HE1	1.85	0.41
1:E:436:ASP:OD2	1:E:439:ARG:HG3	2.20	0.41
1:H:43:SER:HB3	1:H:131:ARG:CZ	2.50	0.41
1:E:451:TRP:CH2	2:F:19:PRO:HD3	2.55	0.41
2:C:25:GLN:HB2	5:C:472:HOH:O	2.20	0.41
1:B:451:TRP:CH2	2:C:19:PRO:HD3	2.55	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:213:ARG:HA	1:B:213:ARG:HD3	1.85	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
2:I:9:LEU:HA	2:I:9:LEU:HD22	1.90	0.41
1:H:451:TRP:CH2	2:I:19:PRO:HD3	2.55	0.41
2:F:113:ILE:HG22	2:F:114:SER:N	2.35	0.41
2:S:113:ILE:HG22	2:S:114:SER:N	2.35	0.41
1:E:251:MET:HB3	1:E:251:MET:HE2	1.88	0.41
2:F:96:ASN:HD21	2:I:7:LEU:HD11	1.86	0.41
1:L:451:TRP:CH2	2:S:19:PRO:HD3	2.55	0.41
1:H:436:ASP:OD2	1:H:439:ARG:HG3	2.21	0.41
1:B:338:GLU:N	5:B:673:HOH:O	2.54	0.41
1:E:175:LYS:HG3	1:E:407:LEU:HD12	2.03	0.41
1:B:175:LYS:HG3	1:B:407:LEU:HD12	2.03	0.41
2:S:25:GLN:HB2	5:S:162:HOH:O	2.20	0.41
1:B:184:ASN:ND2	5:B:519:HOH:O	2.54	0.41
1:E:241:ASN:ND2	1:E:243:THR:H	2.19	0.41
2:C:113:ILE:HG22	2:C:114:SER:N	2.35	0.41
1:H:88:GLU:HA	1:H:89:PRO:HD3	1.95	0.41
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:175:LYS:HG3	1:L:407:LEU:HD12	2.03	0.40
1:L:241:ASN:ND2	1:L:243:THR:H	2.19	0.40
1:H:175:LYS:HG3	1:H:407:LEU:HD12	2.03	0.40
1:E:292:HIS:HA	1:E:325:HIS:HB2	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:292:HIS:HA	1:B:325:HIS:HB2	2.03	0.40
2:I:4:TRP:HA	2:I:5:PRO:HD3	1.89	0.40
2:I:113:ILE:HG22	2:I:114:SER:N	2.35	0.40
1:H:241:ASN:ND2	1:H:243:THR:H	2.19	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 (20) 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	Distance(Å)	Clash(Å)
5:L:480:HOH:O	5:E:488:HOH:O[3_555]	0.08	2.12
5:L:645:HOH:O	5:E:653:HOH:O[3_555]	0.19	2.01
5:L:613:HOH:O	5:E:621:HOH:O[3_555]	0.77	1.43
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
5:E:582:HOH:O	5:H:585:HOH:O[3_555]	1.44	0.76
5:L:574:HOH:O	5:B:582:HOH:O[3_555]	1.46	0.74
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%)	38	38
1	E	433/475 (91%)	416 (96%)	15 (4%)	2 (0%)	38	38
1	H	433/475 (91%)	416 (96%)	15 (4%)	2 (0%)	38	38
1	L	433/475 (91%)	416 (96%)	15 (4%)	2 (0%)	38	38
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%)	43	45

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%)	52	63
1	E	355/385 (92%)	344 (97%)	11 (3%)	52	63
1	H	355/385 (92%)	344 (97%)	11 (3%)	52	63
1	L	355/385 (92%)	344 (97%)	11 (3%)	52	63
2	C	112/112 (100%)	106 (95%)	6 (5%)	31	35
2	F	112/112 (100%)	106 (95%)	6 (5%)	31	35
2	I	112/112 (100%)	106 (95%)	6 (5%)	31	35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S	112/112 (100%)	106 (95%)	6 (5%)	31	35
All	All	1868/1988 (94%)	1800 (96%)	68 (4%)	47	56

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
2	C	47	ASP
2	C	68	THR
2	C	88	GLU
2	C	92	LYS
1	E	21	LYS
1	E	22	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
1	E	229	GLN
1	E	238	HIS
1	E	241	ASN
1	E	267	HIS
1	E	277	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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 chains 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	11,11,12	5.28	2 (18%)	10,12,14	2.36	4 (40%)
1	KCX	E	201	1,3	11,11,12	5.27	2 (18%)	10,12,14	2.37	4 (40%)
1	KCX	H	201	1,3	11,11,12	5.30	2 (18%)	10,12,14	2.36	4 (40%)
1	KCX	L	201	1,3	11,11,12	5.29	2 (18%)	10,12,14	2.37	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
1	KCX	B	201	1,3	-	0/8/10/12	0/0/0/0
1	KCX	E	201	1,3	-	0/8/10/12	0/0/0/0
1	KCX	H	201	1,3	-	0/8/10/12	0/0/0/0
1	KCX	L	201	1,3	-	0/8/10/12	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	201	KCX	O-C	17.30	1.23	1.11
1	L	201	KCX	O-C	17.24	1.23	1.11
1	B	201	KCX	O-C	17.24	1.23	1.11
1	E	201	KCX	O-C	17.21	1.23	1.11
1	L	201	KCX	OQ1-CX	2.17	1.25	1.21
1	H	201	KCX	OQ1-CX	2.16	1.25	1.21
1	B	201	KCX	OQ1-CX	2.15	1.25	1.21
1	E	201	KCX	OQ1-CX	2.14	1.25	1.21

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	201	KCX	OQ2-CX-OQ1	-4.81	116.16	122.17
1	B	201	KCX	OQ2-CX-OQ1	-4.80	116.17	122.17
1	L	201	KCX	OQ2-CX-OQ1	-4.80	116.17	122.17
1	H	201	KCX	OQ2-CX-OQ1	-4.78	116.20	122.17
1	E	201	KCX	OQ2-CX-NZ	3.62	120.84	116.33
1	L	201	KCX	OQ2-CX-NZ	3.62	120.84	116.33
1	B	201	KCX	OQ2-CX-NZ	3.59	120.80	116.33
1	H	201	KCX	OQ2-CX-NZ	3.59	120.80	116.33
1	E	201	KCX	C-CA-N	2.85	116.67	113.83
1	B	201	KCX	C-CA-N	2.83	116.66	113.83

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	201	KCX	C-CA-N	2.82	116.65	113.83
1	H	201	KCX	C-CA-N	2.81	116.64	113.83
1	H	201	KCX	OQ1-CX-NZ	-2.07	121.50	124.94
1	L	201	KCX	OQ1-CX-NZ	-2.06	121.50	124.94
1	B	201	KCX	OQ1-CX-NZ	-2.05	121.53	124.94
1	E	201	KCX	OQ1-CX-NZ	-2.05	121.53	124.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	10,10,10	3.00	3 (30%)	14,14,14	1.94	6 (42%)
4	3PG	B	478	-	10,10,10	1.54	3 (30%)	14,14,14	3.84	7 (50%)
4	3PG	E	477	3	10,10,10	3.01	3 (30%)	14,14,14	1.94	6 (42%)
4	3PG	E	478	-	10,10,10	1.53	3 (30%)	14,14,14	3.84	7 (50%)
4	3PG	H	477	3	10,10,10	3.00	3 (30%)	14,14,14	1.94	6 (42%)
4	3PG	H	478	-	10,10,10	1.53	3 (30%)	14,14,14	3.84	7 (50%)
4	3PG	L	477	3	10,10,10	3.00	3 (30%)	14,14,14	1.94	6 (42%)
4	3PG	L	478	-	10,10,10	1.53	3 (30%)	14,14,14	3.84	7 (50%)

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	477	3PG	C3-C2	7.03	1.64	1.51
4	E	477	3PG	C3-C2	7.01	1.64	1.51
4	H	477	3PG	C3-C2	7.01	1.64	1.51
4	L	477	3PG	C3-C2	7.00	1.64	1.51
4	E	477	3PG	C2-C1	4.91	1.60	1.52
4	L	477	3PG	C2-C1	4.87	1.59	1.52
4	H	477	3PG	C2-C1	4.86	1.59	1.52
4	B	477	3PG	C2-C1	4.84	1.59	1.52
4	E	477	3PG	P-O1P	2.78	1.69	1.60
4	L	477	3PG	P-O1P	2.77	1.69	1.60
4	B	477	3PG	P-O1P	2.77	1.69	1.60
4	H	477	3PG	P-O1P	2.76	1.69	1.60
4	B	478	3PG	P-O1P	2.61	1.69	1.60
4	L	478	3PG	P-O1P	2.60	1.69	1.60
4	H	478	3PG	P-O1P	2.60	1.69	1.60
4	E	478	3PG	P-O1P	2.58	1.69	1.60
4	B	478	3PG	C3-C2	-2.53	1.46	1.51
4	E	478	3PG	C3-C2	-2.52	1.46	1.51
4	L	478	3PG	C3-C2	-2.48	1.47	1.51
4	H	478	3PG	C3-C2	-2.48	1.47	1.51
4	B	478	3PG	C2-C1	2.37	1.56	1.52
4	L	478	3PG	C2-C1	2.35	1.56	1.52
4	H	478	3PG	C2-C1	2.32	1.56	1.52
4	E	478	3PG	C2-C1	2.31	1.56	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	478	3PG	O1P-C3-C2	11.52	136.84	108.63
4	B	478	3PG	O1P-C3-C2	11.51	136.82	108.63
4	H	478	3PG	O1P-C3-C2	11.51	136.81	108.63
4	L	478	3PG	O1P-C3-C2	11.50	136.81	108.63
4	H	478	3PG	O3-C2-C3	-4.44	99.20	109.77
4	E	478	3PG	O3-C2-C3	-4.44	99.19	109.77
4	L	478	3PG	O3-C2-C3	-4.43	99.21	109.77
4	B	478	3PG	O3-C2-C3	-4.42	99.23	109.77
4	L	478	3PG	O2-C1-C2	3.48	122.55	113.19
4	B	478	3PG	O2-C1-C2	3.48	122.54	113.19
4	E	478	3PG	O2-C1-C2	3.47	122.53	113.19
4	H	478	3PG	O2-C1-C2	3.47	122.51	113.19
4	B	477	3PG	O2-C1-C2	3.40	122.33	113.19
4	H	477	3PG	O2-C1-C2	3.40	122.33	113.19
4	L	477	3PG	O2-C1-C2	3.39	122.30	113.19
4	E	477	3PG	O2-C1-C2	3.38	122.30	113.19
4	B	477	3PG	O2-C1-O1	-3.09	117.09	124.07
4	L	478	3PG	P-O1P-C3	-3.08	109.28	118.19
4	E	478	3PG	P-O1P-C3	-3.08	109.29	118.19
4	B	478	3PG	P-O1P-C3	-3.08	109.29	118.19
4	H	477	3PG	O2-C1-O1	-3.08	117.12	124.07
4	L	477	3PG	O2-C1-O1	-3.07	117.12	124.07
4	H	478	3PG	P-O1P-C3	-3.07	109.32	118.19
4	E	477	3PG	O2-C1-O1	-3.06	117.16	124.07
4	H	478	3PG	O1P-P-O2P	-2.94	98.08	106.71
4	L	478	3PG	O1P-P-O2P	-2.93	98.11	106.71
4	B	478	3PG	O1P-P-O2P	-2.93	98.12	106.71
4	E	478	3PG	O1P-P-O2P	-2.92	98.15	106.71
4	B	477	3PG	O4P-P-O1P	-2.62	99.42	106.65
4	L	477	3PG	O4P-P-O1P	-2.61	99.45	106.65
4	E	477	3PG	O4P-P-O1P	-2.60	99.46	106.65
4	H	477	3PG	O4P-P-O1P	-2.59	99.50	106.65
4	E	478	3PG	O2-C1-O1	-2.56	118.28	124.07
4	L	478	3PG	O2-C1-O1	-2.56	118.29	124.07
4	H	478	3PG	O2-C1-O1	-2.55	118.30	124.07
4	B	478	3PG	O2-C1-O1	-2.55	118.31	124.07
4	E	477	3PG	O3-C2-C3	-2.24	104.43	109.77
4	L	477	3PG	O3-C2-C3	-2.23	104.45	109.77
4	B	477	3PG	O3-C2-C3	-2.23	104.46	109.77
4	H	477	3PG	O3-C2-C3	-2.22	104.47	109.77
4	E	477	3PG	O4P-P-O3P	2.15	115.99	107.61
4	H	477	3PG	O4P-P-O3P	2.15	115.98	107.61
4	L	477	3PG	O4P-P-O3P	2.14	115.96	107.61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	477	3PG	O4P-P-O3P	2.14	115.94	107.61
4	E	477	3PG	O3P-P-O1P	-2.08	100.90	106.65
4	B	477	3PG	O3P-P-O1P	-2.07	100.92	106.65
4	L	477	3PG	O3P-P-O1P	-2.07	100.93	106.65
4	B	478	3PG	O4P-P-O2P	2.07	117.21	110.44
4	L	478	3PG	O4P-P-O2P	2.06	117.19	110.44
4	H	477	3PG	O3P-P-O1P	-2.06	100.95	106.65
4	H	478	3PG	O4P-P-O2P	2.06	117.18	110.44
4	E	478	3PG	O4P-P-O2P	2.05	117.15	110.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	B	438/475 (92%)	-0.31	9 (2%) 60 61	4, 13, 36, 50	0
1	E	438/475 (92%)	-0.43	8 (1%) 65 66	4, 13, 36, 50	0
1	H	438/475 (92%)	-0.50	5 (1%) 77 78	4, 13, 36, 50	0
1	L	438/475 (92%)	-0.44	9 (2%) 60 61	4, 13, 36, 50	0
2	C	123/123 (100%)	0.16	5 (4%) 35 36	9, 26, 40, 47	0
2	F	123/123 (100%)	-0.01	3 (2%) 56 56	9, 26, 40, 47	0
2	I	123/123 (100%)	-0.03	5 (4%) 35 36	9, 26, 40, 47	0
2	S	123/123 (100%)	0.24	9 (7%) 15 14	9, 26, 40, 47	0
All	All	2244/2392 (93%)	-0.31	53 (2%) 56 56	4, 17, 39, 50	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	121	ALA	5.9
1	H	22	LEU	5.7
1	B	22	LEU	5.5
1	B	332	VAL	5.2
1	L	22	LEU	5.2
2	F	121	ALA	4.9
1	E	92	GLY	4.8
2	S	122	GLY	4.5
1	L	94	GLU	4.3
1	E	22	LEU	4.1
2	S	121	ALA	3.9
1	E	21	LYS	3.9
1	B	439	ARG	3.8
2	C	121	ALA	3.5
1	E	439	ARG	3.5
1	B	450	LYS	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	L	332	VAL	3.3
1	H	332	VAL	3.2
1	B	451	TRP	3.1
1	E	94	GLU	3.0
1	L	21	LYS	3.0
1	B	68	THR	2.9
1	L	439	ARG	2.8
1	B	94	GLU	2.8
2	I	48	HIS	2.7
1	B	21	LYS	2.7
1	L	68	THR	2.6
1	H	92	GLY	2.6
2	F	122	GLY	2.6
1	H	439	ARG	2.5
2	C	76	GLY	2.4
2	S	108	ARG	2.4
1	E	332	VAL	2.4
1	L	92	GLY	2.3
1	B	331	VAL	2.3
2	S	81	ALA	2.3
1	L	66	TRP	2.2
2	F	92	LYS	2.2
2	S	107	ASN	2.2
1	L	67	THR	2.2
1	E	68	THR	2.2
1	E	66	TRP	2.1
2	S	92	LYS	2.1
2	S	123	TYR	2.1
2	C	48	HIS	2.1
2	I	8	ASN	2.1
2	I	122	GLY	2.1
2	C	23	THR	2.1
2	S	77	CYS	2.1
2	S	120	PRO	2.0
1	H	21	LYS	2.0
2	I	123	TYR	2.0
2	C	2	GLN	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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	KCX	E	201	12/13	0.13	1.66	6,17,29,35	0
1	KCX	L	201	12/13	0.12	1.15	6,17,29,35	0
1	KCX	H	201	12/13	0.11	0.88	6,17,29,35	0
1	KCX	B	201	12/13	0.13	0.82	6,17,29,35	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	3PG	H	478	11/11	0.21	4.33	41,44,47,49	0
4	3PG	E	478	11/11	0.22	3.77	41,44,47,49	0
3	MG	E	476	1/1	0.20	3.75	29,29,29,29	0
4	3PG	B	478	11/11	0.25	3.68	41,44,47,49	0
4	3PG	L	478	11/11	0.19	3.48	41,44,47,49	0
4	3PG	L	477	11/11	0.19	1.60	35,38,43,46	0
4	3PG	E	477	11/11	0.19	1.09	35,38,43,46	0
4	3PG	H	477	11/11	0.16	1.06	35,38,43,46	0
3	MG	B	476	1/1	0.13	1.00	29,29,29,29	0
3	MG	L	476	1/1	0.13	0.96	29,29,29,29	0
4	3PG	B	477	11/11	0.16	0.57	35,38,43,46	0
3	MG	H	476	1/1	0.09	-0.66	29,29,29,29	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.