



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:30 PM GMT

PDB ID : 1XKL
Title : Crystal Structure of Salicylic Acid-binding Protein 2 (SABP2) from *Nicotiana tabacum*, NESG Target AR2241
Authors : Forouhar, F.; Chen, Y.; Chiang, Y.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2004-09-29
Resolution : 2.00 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

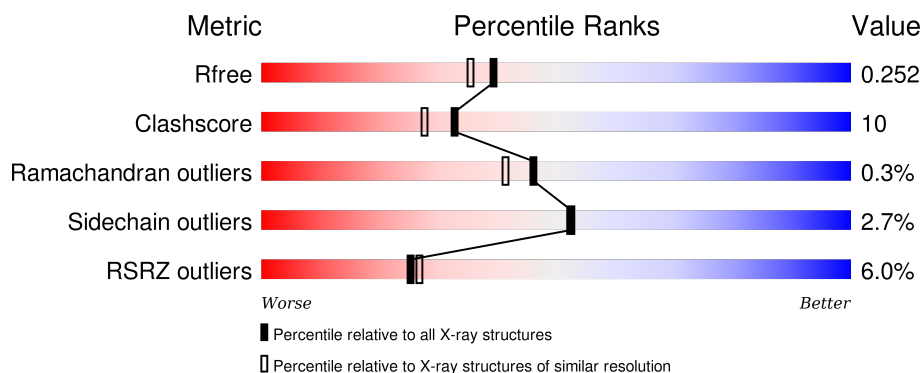
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	273	
1	B	273	
1	C	273	
1	D	273	

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	STH	A	297	X	-	-	-
2	STH	B	298	X	-	-	-
2	STH	C	299	X	-	-	-
2	STH	D	300	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9105 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 salicylic acid-binding protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	Se	0	0	0
			2042	1317	331	380	5	9			
1	B	256	Total	C	N	O	S	Se	0	0	0
			2022	1304	328	376	5	9			
1	C	257	Total	C	N	O	S	Se	0	0	0
			2034	1313	329	378	5	9			
1	D	257	Total	C	N	O	S	Se	0	0	0
			2033	1311	329	379	5	9			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
A	66	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
A	85	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
A	91	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
A	108	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
A	149	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
A	183	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
A	239	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
A	241	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
A	261	MET	-	CLONING ARTIFACT	UNP Q6RYA0
A	262	ALA	-	CLONING ARTIFACT	UNP Q6RYA0
A	263	GLY	-	CLONING ARTIFACT	UNP Q6RYA0
A	264	ASP	-	CLONING ARTIFACT	UNP Q6RYA0
A	265	PRO	-	CLONING ARTIFACT	UNP Q6RYA0
A	266	LEU	-	CLONING ARTIFACT	UNP Q6RYA0
A	267	GLU	-	CLONING ARTIFACT	UNP Q6RYA0
A	268	HIS	-	EXPRESSION TAG	UNP Q6RYA0
A	269	HIS	-	EXPRESSION TAG	UNP Q6RYA0
A	270	HIS	-	EXPRESSION TAG	UNP Q6RYA0
A	271	HIS	-	EXPRESSION TAG	UNP Q6RYA0
A	272	HIS	-	EXPRESSION TAG	UNP Q6RYA0

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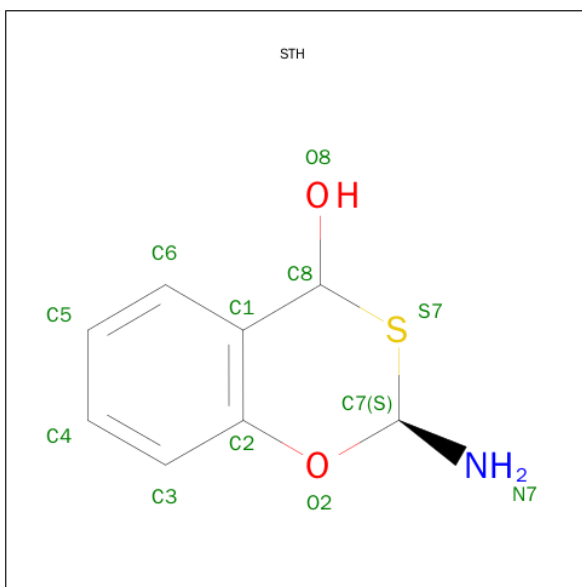
Chain	Residue	Modelled	Actual	Comment	Reference
A	273	HIS	-	EXPRESSION TAG	UNP Q6RYA0
B	63	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
B	66	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
B	85	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
B	91	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
B	108	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
B	149	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
B	183	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
B	239	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
B	241	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
B	261	MET	-	CLONING ARTIFACT	UNP Q6RYA0
B	262	ALA	-	CLONING ARTIFACT	UNP Q6RYA0
B	263	GLY	-	CLONING ARTIFACT	UNP Q6RYA0
B	264	ASP	-	CLONING ARTIFACT	UNP Q6RYA0
B	265	PRO	-	CLONING ARTIFACT	UNP Q6RYA0
B	266	LEU	-	CLONING ARTIFACT	UNP Q6RYA0
B	267	GLU	-	CLONING ARTIFACT	UNP Q6RYA0
B	268	HIS	-	EXPRESSION TAG	UNP Q6RYA0
B	269	HIS	-	EXPRESSION TAG	UNP Q6RYA0
B	270	HIS	-	EXPRESSION TAG	UNP Q6RYA0
B	271	HIS	-	EXPRESSION TAG	UNP Q6RYA0
B	272	HIS	-	EXPRESSION TAG	UNP Q6RYA0
B	273	HIS	-	EXPRESSION TAG	UNP Q6RYA0
C	63	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
C	66	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
C	85	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
C	91	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
C	108	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
C	149	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
C	183	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
C	239	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
C	241	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
C	261	MET	-	CLONING ARTIFACT	UNP Q6RYA0
C	262	ALA	-	CLONING ARTIFACT	UNP Q6RYA0
C	263	GLY	-	CLONING ARTIFACT	UNP Q6RYA0
C	264	ASP	-	CLONING ARTIFACT	UNP Q6RYA0
C	265	PRO	-	CLONING ARTIFACT	UNP Q6RYA0
C	266	LEU	-	CLONING ARTIFACT	UNP Q6RYA0
C	267	GLU	-	CLONING ARTIFACT	UNP Q6RYA0
C	268	HIS	-	EXPRESSION TAG	UNP Q6RYA0
C	269	HIS	-	EXPRESSION TAG	UNP Q6RYA0
C	270	HIS	-	EXPRESSION TAG	UNP Q6RYA0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	271	HIS	-	EXPRESSION TAG	UNP Q6RYA0
C	272	HIS	-	EXPRESSION TAG	UNP Q6RYA0
C	273	HIS	-	EXPRESSION TAG	UNP Q6RYA0
D	63	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
D	66	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
D	85	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
D	91	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
D	108	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
D	149	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
D	183	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
D	239	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
D	241	MSE	MET	MODIFIED RESIDUE	UNP Q6RYA0
D	261	MET	-	CLONING ARTIFACT	UNP Q6RYA0
D	262	ALA	-	CLONING ARTIFACT	UNP Q6RYA0
D	263	GLY	-	CLONING ARTIFACT	UNP Q6RYA0
D	264	ASP	-	CLONING ARTIFACT	UNP Q6RYA0
D	265	PRO	-	CLONING ARTIFACT	UNP Q6RYA0
D	266	LEU	-	CLONING ARTIFACT	UNP Q6RYA0
D	267	GLU	-	CLONING ARTIFACT	UNP Q6RYA0
D	268	HIS	-	EXPRESSION TAG	UNP Q6RYA0
D	269	HIS	-	EXPRESSION TAG	UNP Q6RYA0
D	270	HIS	-	EXPRESSION TAG	UNP Q6RYA0
D	271	HIS	-	EXPRESSION TAG	UNP Q6RYA0
D	272	HIS	-	EXPRESSION TAG	UNP Q6RYA0
D	273	HIS	-	EXPRESSION TAG	UNP Q6RYA0

- Molecule 2 is 2-AMINO-4H-1,3-BENZOXATHIIN-4-OL (three-letter code: STH) (formula: C₈H₉NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	B	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	C	1	Total	C	N	O	S	0	0
			12	8	1	2	1		
2	D	1	Total	C	N	O	S	0	0
			12	8	1	2	1		

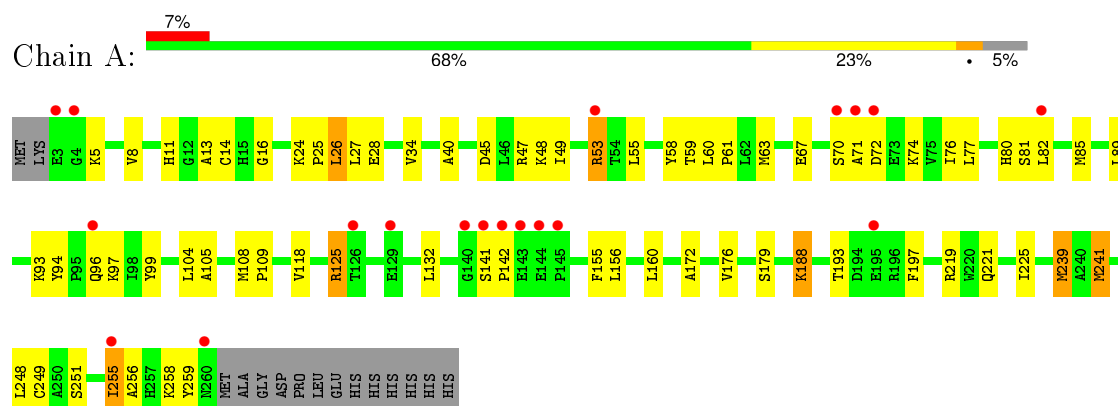
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	204	Total	O	0	0
			204	204		
3	B	238	Total	O	0	0
			238	238		
3	C	243	Total	O	0	0
			243	243		
3	D	241	Total	O	0	0
			241	241		

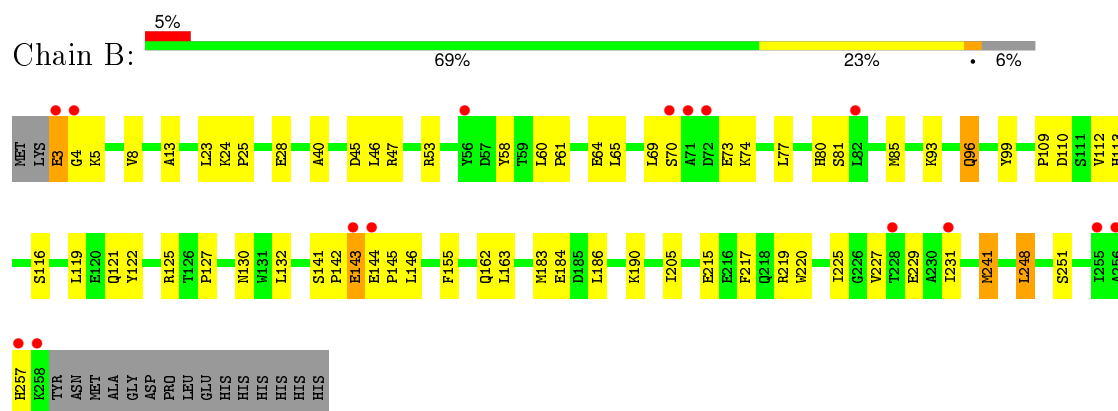
3 Residue-property plots [i](#)

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.

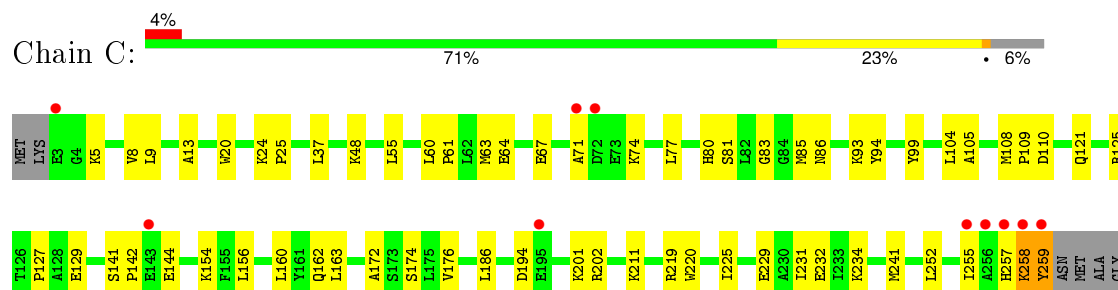
• Molecule 1: salicylic acid-binding protein 2



• Molecule 1: salicylic acid-binding protein 2

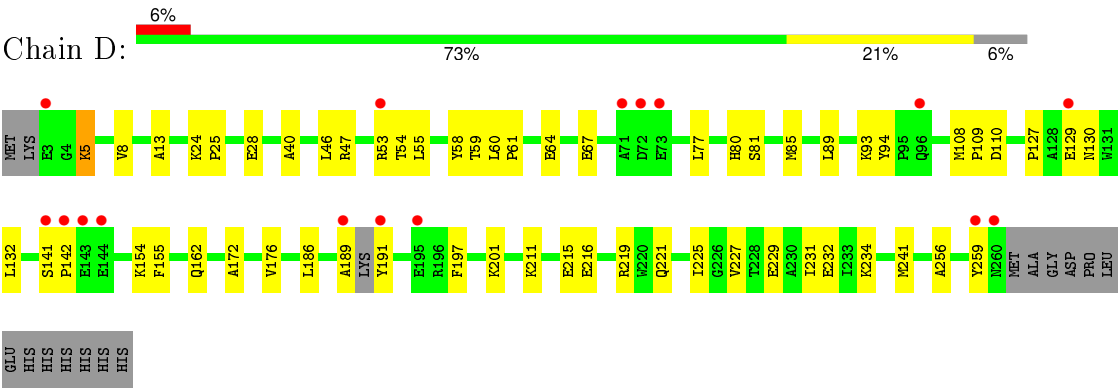


• Molecule 1: salicylic acid-binding protein 2



ASP
PRO
LEU
GLU
HIS
HIS
HIS
HIS
HIS

• Molecule 1: salicylic acid-binding protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	136.46Å 167.77Å 44.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.15 – 2.00 29.84 – 1.99	Depositor EDS
% Data completeness (in resolution range)	84.2 (27.15-2.00) 95.4 (29.84-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.190 , 0.234 0.209 , 0.252	Depositor DCC
R_{free} test set	6491 reflections (10.86%)	DCC
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 131273 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9105	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: STH

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	0.36	1/2085 (0.0%)	0.59	1/2808 (0.0%)
1	B	0.35	1/2064 (0.0%)	0.58	1/2779 (0.0%)
1	C	0.37	1/2077 (0.0%)	0.59	1/2797 (0.0%)
1	D	0.35	1/2075 (0.0%)	0.56	1/2794 (0.0%)
All	All	0.36	4/8301 (0.0%)	0.58	4/11178 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	81	SER	N-CA	-5.87	1.34	1.46
1	D	81	SER	N-CA	-5.71	1.34	1.46
1	B	81	SER	N-CA	-5.60	1.35	1.46
1	A	81	SER	N-CA	-5.37	1.35	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	SER	CA-CB-OG	6.32	128.26	111.20
1	B	81	SER	CA-CB-OG	6.26	128.12	111.20
1	C	81	SER	CA-CB-OG	6.24	128.06	111.20
1	D	81	SER	CA-CB-OG	6.19	127.91	111.20

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	2042	0	2014	52	0
1	B	2022	0	1999	42	0
1	C	2034	0	2008	39	0
1	D	2033	0	2000	39	0
2	A	12	0	6	1	0
2	B	12	0	6	1	0
2	C	12	0	6	1	0
2	D	12	0	7	1	0
3	A	204	0	0	2	0
3	B	238	0	0	3	0
3	C	243	0	0	2	1
3	D	241	0	0	4	1
All	All	9105	0	8046	169	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (169) 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:A:53:ARG:HB3	1:A:53:ARG:HH11	1.30	0.96
1:C:194:ASP:HB2	3:C:533:HOH:O	1.70	0.92
1:A:160:LEU:HB3	1:A:239:MSE:HE1	1.56	0.85
1:A:160:LEU:HB3	1:A:239:MSE:CE	2.08	0.83
1:D:85:MSE:SE	1:D:109:PRO:HG3	2.29	0.82
1:B:85:MSE:SE	1:B:109:PRO:HG3	2.30	0.81
1:A:85:MSE:SE	1:A:109:PRO:HG3	2.35	0.77
1:A:108:MSE:O	1:A:225:ILE:HD13	1.89	0.73
1:D:55:LEU:HD22	1:D:186:LEU:HD21	1.71	0.72
1:A:67:GLU:HG3	1:A:94:TYR:OH	1.88	0.72
1:B:23:LEU:HD22	1:B:248:LEU:HD13	1.74	0.70
1:D:5:LYS:HD3	1:D:256:ALA:HB1	1.75	0.69
1:D:108:MSE:H	1:D:221:GLN:HE22	1.41	0.68
1:D:132:LEU:HD12	1:D:155:PHE:HA	1.75	0.68
1:B:70:SER:HB2	1:B:73:GLU:HB2	1.78	0.65
1:C:24:LYS:HB3	1:C:25:PRO:HD3	1.78	0.65
1:B:24:LYS:HB3	1:B:25:PRO:HD3	1.79	0.65
1:D:53:ARG:HG3	1:D:54:THR:HG23	1.79	0.65
1:C:85:MSE:SE	1:C:109:PRO:HG3	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:LEU:HD23	1:C:255:ILE:HD11	1.78	0.63
1:B:145:PRO:HG2	1:B:184:GLU:HG3	1.82	0.61
1:A:70:SER:O	1:A:71:ALA:HB3	2.01	0.60
1:D:60:LEU:HB3	1:D:61:PRO:HD3	1.83	0.60
1:C:162:GLN:NE2	1:C:211:LYS:HD3	2.16	0.60
1:B:60:LEU:O	1:B:64:GLU:HG3	2.02	0.60
1:D:108:MSE:H	1:D:221:GLN:NE2	1.99	0.60
1:B:205:ILE:HG12	1:B:231:ILE:CG2	2.30	0.60
1:C:37:LEU:HD23	1:C:37:LEU:H	1.67	0.59
1:A:24:LYS:HB3	1:A:25:PRO:HD3	1.85	0.59
1:C:172:ALA:O	1:C:176:VAL:HG13	2.02	0.58
1:C:156:LEU:HD23	1:C:160:LEU:HD12	1.84	0.58
1:A:221:GLN:HB3	1:A:225:ILE:HD12	1.85	0.58
1:A:96:GLN:HB3	3:A:334:HOH:O	2.03	0.58
1:B:132:LEU:HD12	1:B:155:PHE:HA	1.86	0.58
1:B:53:ARG:HE	1:B:146:LEU:CD1	2.17	0.57
1:C:141:SER:HB2	1:C:142:PRO:HD2	1.85	0.57
1:D:60:LEU:O	1:D:64:GLU:HG3	2.04	0.57
1:C:71:ALA:HA	3:C:362:HOH:O	2.06	0.56
1:A:8:VAL:HB	1:A:77:LEU:HD23	1.88	0.56
1:B:96:GLN:H	1:B:96:GLN:CD	2.07	0.56
1:A:141:SER:HB2	1:A:142:PRO:HD2	1.87	0.56
1:D:24:LYS:HB3	1:D:25:PRO:HD3	1.88	0.56
1:C:121:GLN:O	1:C:125:ARG:HG3	2.06	0.56
1:D:201:LYS:HD3	1:D:259:TYR:CD2	2.42	0.55
1:C:129:GLU:H	1:C:129:GLU:CD	2.07	0.55
1:D:234:LYS:C	1:D:234:LYS:HD3	2.27	0.55
1:B:145:PRO:HG2	1:B:184:GLU:CG	2.36	0.54
1:C:80:HIS:CG	1:C:241:MSE:HE1	2.42	0.54
1:A:251:SER:O	1:A:255:ILE:HG23	2.08	0.54
1:B:3:GLU:CD	1:B:4:GLY:H	2.12	0.53
1:D:229:GLU:OE2	1:D:231:ILE:HD11	2.08	0.53
1:A:53:ARG:HB3	1:A:53:ARG:NH1	2.11	0.53
1:A:255:ILE:HG13	1:A:256:ALA:N	2.23	0.53
1:A:160:LEU:HB3	1:A:239:MSE:HE3	1.88	0.53
1:C:60:LEU:HB3	1:C:61:PRO:HD3	1.89	0.53
1:B:8:VAL:HB	1:B:77:LEU:HD23	1.91	0.52
1:B:141:SER:HB2	1:B:142:PRO:HD2	1.91	0.52
1:B:110:ASP:HA	1:B:225:ILE:HD12	1.91	0.52
1:B:231:ILE:HD13	1:B:251:SER:HB3	1.92	0.52
1:A:24:LYS:O	1:A:28:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LEU:HB3	1:B:61:PRO:HD3	1.92	0.52
1:D:201:LYS:HD3	1:D:259:TYR:HD2	1.75	0.52
1:B:190:LYS:HE2	3:B:465:HOH:O	2.09	0.51
1:A:5:LYS:HD2	1:A:76:ILE:HD11	1.93	0.51
1:B:215:GLU:O	1:B:219:ARG:HG2	2.10	0.51
1:C:121:GLN:HG3	1:C:220:TRP:CH2	2.46	0.50
1:A:55:LEU:HD23	1:A:89:LEU:HD11	1.93	0.50
1:D:40:ALA:HB3	1:D:58:TYR:HA	1.93	0.50
1:C:13:ALA:HB3	2:C:299:STH:S7	2.51	0.50
1:D:8:VAL:HB	1:D:77:LEU:HD23	1.92	0.50
1:D:80:HIS:CG	1:D:241:MSE:HE1	2.46	0.50
1:B:24:LYS:O	1:B:28:GLU:HG3	2.11	0.50
1:B:112:VAL:HG11	3:B:510:HOH:O	2.10	0.50
1:D:24:LYS:O	1:D:28:GLU:HG3	2.11	0.49
1:D:108:MSE:HE3	1:D:225:ILE:HB	1.93	0.49
1:C:8:VAL:HB	1:C:77:LEU:HD23	1.94	0.49
1:A:188:LYS:NZ	1:A:188:LYS:HB3	2.27	0.49
1:A:71:ALA:HA	1:A:97:LYS:HD3	1.95	0.49
1:C:74:LYS:HB2	1:C:99:TYR:CZ	2.48	0.48
1:D:13:ALA:HB3	2:D:300:STH:S7	2.53	0.48
1:A:108:MSE:O	1:A:118:VAL:HG11	2.14	0.48
1:B:70:SER:HB2	1:B:73:GLU:CB	2.43	0.48
1:A:125:ARG:HB3	3:A:377:HOH:O	2.12	0.48
1:A:13:ALA:HB1	1:A:179:SER:OG	2.14	0.48
1:B:145:PRO:CG	1:B:184:GLU:HG3	2.44	0.48
1:A:74:LYS:HB2	1:A:99:TYR:CZ	2.49	0.48
1:A:48:LYS:HE3	1:B:46:LEU:HD13	1.95	0.47
1:D:93:LYS:HD3	3:D:429:HOH:O	2.13	0.47
1:D:55:LEU:HD23	1:D:89:LEU:HD11	1.96	0.47
1:A:59:THR:HG22	1:A:59:THR:O	2.15	0.47
1:D:108:MSE:SE	1:D:227:VAL:HG12	2.65	0.47
1:D:85:MSE:HE2	1:D:186:LEU:HD13	1.96	0.47
1:C:127:PRO:HB2	1:C:129:GLU:OE2	2.15	0.47
1:D:162:GLN:NE2	1:D:211:LYS:HG3	2.30	0.47
1:A:172:ALA:O	1:A:176:VAL:HG13	2.15	0.47
1:A:80:HIS:CG	1:A:241:MSE:HE1	2.50	0.47
1:D:108:MSE:HA	1:D:109:PRO:HD3	1.74	0.46
1:B:13:ALA:HB3	2:B:298:STH:S7	2.55	0.46
1:D:189:ALA:HB3	1:D:191:TYR:CZ	2.50	0.46
1:A:60:LEU:HB3	1:A:61:PRO:HD3	1.97	0.46
1:D:67:GLU:HB2	1:D:94:TYR:OH	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:GLN:HG2	1:C:163:LEU:HG	1.98	0.46
1:B:119:LEU:HB3	1:B:183:MSE:SE	2.65	0.46
1:C:67:GLU:HG2	1:C:94:TYR:OH	2.16	0.46
1:A:156:LEU:HD23	1:A:160:LEU:HD12	1.98	0.46
1:A:132:LEU:HD12	1:A:155:PHE:HA	1.97	0.46
1:A:258:LYS:HG3	1:A:259:TYR:CD1	2.51	0.46
1:D:141:SER:HB2	1:D:142:PRO:HD2	1.98	0.46
1:B:122:TYR:HB2	1:B:217:PHE:CZ	2.51	0.45
1:A:49:ILE:HD13	1:A:179:SER:HA	1.99	0.45
1:D:127:PRO:HG2	1:D:130:ASN:OD1	2.16	0.45
1:C:48:LYS:HG2	1:D:46:LEU:HD13	1.97	0.45
1:B:116:SER:HB3	1:B:186:LEU:HB3	1.99	0.45
1:A:104:LEU:O	1:A:105:ALA:C	2.55	0.45
1:B:40:ALA:HB3	1:B:58:TYR:HA	1.99	0.45
1:B:93:LYS:NZ	1:C:64:GLU:HG2	2.32	0.45
1:B:65:LEU:O	1:B:69:LEU:HD13	2.17	0.45
1:A:63:MSE:HE1	1:A:93:LYS:HB2	1.99	0.44
1:A:26:LEU:HB3	1:A:249:CYS:SG	2.56	0.44
1:A:40:ALA:HB3	1:A:58:TYR:HA	1.99	0.44
1:A:13:ALA:O	1:A:14:CYS:HB2	2.17	0.44
1:A:63:MSE:CE	1:A:93:LYS:HG3	2.48	0.44
1:A:70:SER:C	1:A:72:ASP:H	2.21	0.44
1:C:234:LYS:NZ	1:C:234:LYS:HB2	2.33	0.44
1:C:202:ARG:NH1	1:C:225:ILE:HG12	2.33	0.44
1:A:70:SER:HB2	1:A:72:ASP:OD2	2.18	0.44
1:A:70:SER:O	1:A:71:ALA:CB	2.66	0.43
1:C:231:ILE:HG22	1:C:232:GLU:N	2.33	0.43
1:C:108:MSE:HA	1:C:109:PRO:HD3	1.82	0.43
1:D:231:ILE:HG22	1:D:232:GLU:N	2.32	0.43
1:B:121:GLN:HG3	1:B:220:TRP:CH2	2.54	0.43
1:A:118:VAL:HG12	1:A:225:ILE:HD11	2.01	0.43
1:C:37:LEU:CD2	1:C:37:LEU:H	2.30	0.43
1:B:74:LYS:HB2	1:B:99:TYR:CE1	2.53	0.43
1:D:172:ALA:O	1:D:176:VAL:HG13	2.19	0.42
1:A:108:MSE:HA	1:A:109:PRO:HD3	1.84	0.42
1:A:74:LYS:HB2	1:A:99:TYR:CE1	2.55	0.42
1:D:47:ARG:NH1	3:D:340:HOH:O	2.50	0.42
1:A:45:ASP:OD2	1:A:47:ARG:HB2	2.19	0.42
1:A:82:LEU:HB2	2:A:297:STH:O8	2.19	0.42
1:C:55:LEU:HD22	1:C:186:LEU:HD21	2.00	0.42
1:C:37:LEU:HD23	1:C:37:LEU:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:HIS:CG	1:B:241:MSE:HE1	2.55	0.42
1:C:201:LYS:HE3	1:C:259:TYR:CE2	2.55	0.42
1:C:83:GLY:HA2	1:C:86:ASN:OD1	2.20	0.42
1:D:89:LEU:N	1:D:89:LEU:HD12	2.35	0.41
1:C:241:MSE:H	1:C:241:MSE:SE	2.52	0.41
1:D:59:THR:HG22	1:D:59:THR:O	2.21	0.41
1:C:9:LEU:HB3	1:C:20:TRP:CE2	2.55	0.41
1:A:63:MSE:HE1	1:A:93:LYS:HG3	2.02	0.41
1:D:216:GLU:HG3	3:D:473:HOH:O	2.20	0.41
1:B:3:GLU:CD	1:B:4:GLY:N	2.73	0.41
1:A:27:LEU:HB2	1:A:34:VAL:HG21	2.01	0.41
1:B:113:HIS:HB3	3:B:422:HOH:O	2.20	0.41
1:B:127:PRO:HG2	1:B:130:ASN:OD1	2.19	0.41
1:C:229:GLU:OE2	1:C:258:LYS:HE3	2.20	0.41
1:C:110:ASP:HA	1:C:225:ILE:HD12	2.03	0.41
1:B:143:GLU:H	1:B:143:GLU:HG3	1.55	0.41
1:B:162:GLN:HG2	1:B:163:LEU:HG	2.02	0.41
1:A:193:THR:O	1:A:197:PHE:HB3	2.21	0.41
1:C:104:LEU:O	1:C:105:ALA:C	2.58	0.41
1:C:174:SER:HB2	3:D:378:HOH:O	2.21	0.41
1:B:125:ARG:NH1	1:B:220:TRP:CG	2.87	0.40
1:B:45:ASP:OD2	1:B:47:ARG:HB2	2.21	0.40
1:C:63:MSE:HE3	1:C:93:LYS:HD3	2.03	0.40
1:B:227:VAL:HG22	1:B:229:GLU:H	1.85	0.40
1:A:11:HIS:CD2	1:A:16:GLY:HA2	2.57	0.40
1:D:215:GLU:O	1:D:219:ARG:HG2	2.22	0.40
1:D:110:ASP:HA	1:D:197:PHE:CE2	2.57	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:533:HOH:O	3:D:533:HOH:O[2_665]	1.30	0.90
3:C:542:HOH:O	3:C:542:HOH:O[2_665]	1.51	0.69

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	256/273 (94%)	244 (95%)	12 (5%)	0	100	100
1	B	254/273 (93%)	237 (93%)	16 (6%)	1 (0%)	39	33
1	C	255/273 (93%)	241 (94%)	12 (5%)	2 (1%)	24	15
1	D	253/273 (93%)	245 (97%)	8 (3%)	0	100	100
All	All	1018/1092 (93%)	967 (95%)	48 (5%)	3 (0%)	46	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	257	HIS
1	C	258	LYS
1	C	257	HIS

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	220/224 (98%)	211 (96%)	9 (4%)	37	32
1	B	218/224 (97%)	211 (97%)	7 (3%)	46	44
1	C	219/224 (98%)	214 (98%)	5 (2%)	58	60
1	D	219/224 (98%)	216 (99%)	3 (1%)	74	77
All	All	876/896 (98%)	852 (97%)	24 (3%)	52	52

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	53	ARG
1	A	125	ARG
1	A	188	LYS
1	A	219	ARG
1	A	239	MSE
1	A	241	MSE
1	A	248	LEU
1	A	255	ILE
1	B	3	GLU
1	B	5	LYS
1	B	96	GLN
1	B	143	GLU
1	B	144	GLU
1	B	241	MSE
1	B	248	LEU
1	C	5	LYS
1	C	144	GLU
1	C	154	LYS
1	C	219	ARG
1	C	259	TYR
1	D	5	LYS
1	D	129	GLU
1	D	154	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	B	96	GLN
1	C	130	ASN
1	C	135	GLN
1	D	96	GLN
1	D	114	ASN
1	D	221	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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	$\# Z > 2$
2	STH	A	297	1	9,13,13	4.39	6 (66%)	10,18,18	1.84	1 (10%)
2	STH	B	298	1	9,13,13	4.41	5 (55%)	10,18,18	1.75	1 (10%)
2	STH	C	299	1	9,13,13	4.53	6 (66%)	10,18,18	1.84	1 (10%)
2	STH	D	300	1	9,13,13	4.28	6 (66%)	10,18,18	1.81	1 (10%)

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	STH	A	297	1	1/1/2/2	0/0/12/12	0/1/2/2
2	STH	B	298	1	1/1/2/2	0/0/12/12	0/1/2/2
2	STH	C	299	1	1/1/2/2	0/0/12/12	0/1/2/2
2	STH	D	300	1	1/1/2/2	0/0/12/12	0/1/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	299	STH	C7-S7	-11.04	1.61	1.83
2	B	298	STH	C7-S7	-10.92	1.61	1.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	297	STH	C7-S7	-10.90	1.61	1.83
2	D	300	STH	C7-S7	-10.49	1.62	1.83
2	D	300	STH	C4-C3	2.01	1.43	1.38
2	C	299	STH	C4-C3	2.07	1.43	1.38
2	A	297	STH	C5-C4	2.08	1.43	1.38
2	D	300	STH	C5-C4	2.17	1.43	1.38
2	A	297	STH	C4-C3	2.21	1.43	1.38
2	B	298	STH	C5-C4	2.25	1.43	1.38
2	C	299	STH	C5-C4	2.38	1.44	1.38
2	B	298	STH	O2-C2	2.73	1.42	1.37
2	D	300	STH	O2-C2	2.84	1.42	1.37
2	C	299	STH	O2-C2	2.92	1.42	1.37
2	A	297	STH	O2-C2	2.99	1.42	1.37
2	A	297	STH	C6-C1	3.80	1.44	1.39
2	D	300	STH	C2-C1	4.02	1.48	1.39
2	D	300	STH	C6-C1	4.11	1.45	1.39
2	B	298	STH	C2-C1	4.16	1.48	1.39
2	B	298	STH	C6-C1	4.24	1.45	1.39
2	A	297	STH	C2-C1	4.25	1.48	1.39
2	C	299	STH	C2-C1	4.33	1.49	1.39
2	C	299	STH	C6-C1	4.51	1.45	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	298	STH	O8-C8-C1	5.13	121.30	112.01
2	D	300	STH	O8-C8-C1	5.35	121.71	112.01
2	C	299	STH	O8-C8-C1	5.39	121.77	112.01
2	A	297	STH	O8-C8-C1	5.41	121.82	112.01

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	297	STH	C8
2	D	300	STH	C8
2	B	298	STH	C8
2	C	299	STH	C8

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
2	A	297	STH	1	0
2	B	298	STH	1	0
2	C	299	STH	1	0
2	D	300	STH	1	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	249/273 (91%)	0.41	19 (7%) 17 18	10, 21, 37, 50	0
1	B	247/273 (90%)	0.40	15 (6%) 25 26	10, 21, 38, 53	0
1	C	248/273 (90%)	0.19	10 (4%) 42 44	10, 18, 35, 54	0
1	D	248/273 (90%)	0.47	16 (6%) 22 23	12, 24, 40, 54	0
All	All	992/1092 (90%)	0.37	60 (6%) 25 27	10, 21, 38, 54	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	257	HIS	7.8
1	D	3	GLU	6.6
1	A	71	ALA	5.7
1	A	142	PRO	5.4
1	C	257	HIS	5.1
1	D	142	PRO	5.0
1	C	256	ALA	5.0
1	C	258	LYS	4.9
1	A	143	GLU	4.7
1	A	3	GLU	4.5
1	D	260	ASN	4.4
1	A	140	GLY	4.4
1	C	259	TYR	4.4
1	B	70	SER	4.3
1	A	145	PRO	4.2
1	A	141	SER	3.8
1	B	256	ALA	3.8
1	D	53	ARG	3.7
1	A	144	GLU	3.7
1	B	72	ASP	3.5
1	A	260	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	143	GLU	3.4
1	D	73	GLU	3.2
1	B	258	LYS	3.1
1	D	195	GLU	3.1
1	B	4	GLY	3.1
1	B	144	GLU	3.0
1	C	255	ILE	3.0
1	C	72	ASP	2.9
1	D	141	SER	2.9
1	C	3	GLU	2.9
1	D	143	GLU	2.9
1	D	71	ALA	2.8
1	B	82	LEU	2.7
1	D	259	TYR	2.7
1	A	53	ARG	2.7
1	A	72	ASP	2.6
1	A	82	LEU	2.6
1	B	231	ILE	2.6
1	B	71	ALA	2.4
1	A	4	GLY	2.3
1	A	129	GLU	2.3
1	A	255	ILE	2.3
1	A	70	SER	2.2
1	C	71	ALA	2.2
1	B	228	THR	2.2
1	B	3	GLU	2.2
1	D	191	TYR	2.2
1	B	255	ILE	2.2
1	D	72	ASP	2.1
1	D	96	GLN	2.1
1	C	195	GLU	2.1
1	D	129	GLU	2.1
1	A	96	GLN	2.1
1	A	126	THR	2.1
1	D	144	GLU	2.1
1	D	189	ALA	2.1
1	B	56	TYR	2.0
1	A	195	GLU	2.0
1	B	143	GLU	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(\AA^2)	Q<0.9
2	STH	C	299	12/12	0.92	0.17	1.11	17,19,20,27	0
2	STH	B	298	12/12	0.90	0.17	0.53	21,22,26,27	0
2	STH	D	300	12/12	0.89	0.17	0.43	21,24,26,32	0
2	STH	A	297	12/12	0.93	0.14	-0.10	14,18,19,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.