



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2018 – 01:46 PM EDT

PDB ID : 6D6B
Title : The structure of ligand binding domain of LasR in complex with TP-1 homolog, compound 11
Authors : Dong, S.H.; Nair, S.K.
Deposited on : 2018-04-20
Resolution : 1.70 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031172
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

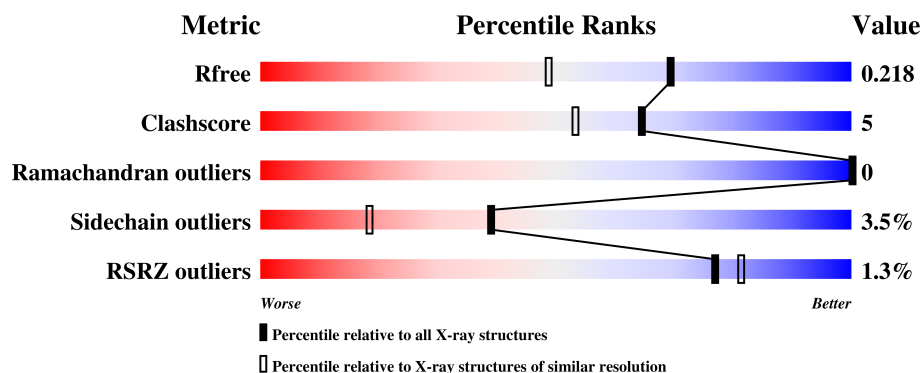
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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.




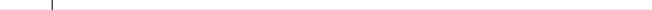

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	3793 (1.70-1.70)
Clashscore	122126	4167 (1.70-1.70)
Ramachandran outliers	120053	4100 (1.70-1.70)
Sidechain outliers	120020	4100 (1.70-1.70)
RSRZ outliers	108989	3718 (1.70-1.70)

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	170	 86% 11% .
1	B	170	 85% 11% ..
1	C	170	 86% 11% ..
1	D	170	 83% 12% . .
1	E	170	 88% 9% . .

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Mol	Chain	Length	Quality of chain		
1	F	170		86%	9% . .
1	G	170		86%	12% ..
1	H	170		85%	12% ...

2 Entry composition

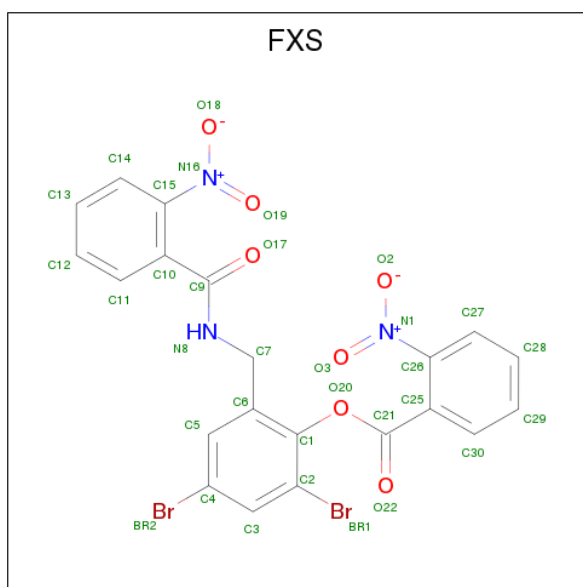
There are 3 unique types of molecules in this entry. The entry contains 11472 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transcriptional activator protein LasR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	2	0
			1312	841	218	248	5			
1	B	166	Total	C	N	O	S	0	2	0
			1312	841	218	248	5			
1	C	166	Total	C	N	O	S	0	2	0
			1310	841	218	246	5			
1	D	163	Total	C	N	O	S	0	2	0
			1287	826	215	241	5			
1	E	165	Total	C	N	O	S	0	2	0
			1304	835	217	247	5			
1	F	164	Total	C	N	O	S	0	2	0
			1297	830	216	246	5			
1	G	168	Total	C	N	O	S	0	2	0
			1326	851	222	248	5			
1	H	166	Total	C	N	O	S	0	2	0
			1310	841	218	246	5			

- Molecule 2 is 2,4-dibromo-6-[[[(2-nitrobenzene-1-carbonyl)amino]methyl]phenyl 2-nitrobenzoate (three-letter code: FXS) (formula: C₂₁H₁₃Br₂N₃O₇).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	0	0
			33	2	21	3	7		
2	B	1	Total	Br	C	N	O	0	0
			33	2	21	3	7		
2	C	1	Total	Br	C	N	O	0	0
			33	2	21	3	7		
2	D	1	Total	Br	C	N	O	0	0
			33	2	21	3	7		
2	E	1	Total	Br	C	N	O	0	0
			33	2	21	3	7		
2	F	1	Total	Br	C	N	O	0	0
			33	2	21	3	7		
2	G	1	Total	Br	C	N	O	0	0
			33	2	21	3	7		
2	H	1	Total	Br	C	N	O	0	0
			33	2	21	3	7		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	92	Total	O	0	0
			92	92		
3	B	85	Total	O	0	0
			85	85		
3	C	103	Total	O	0	0
			103	103		
3	D	72	Total	O	0	0
			72	72		

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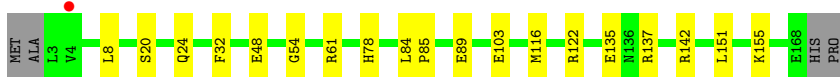
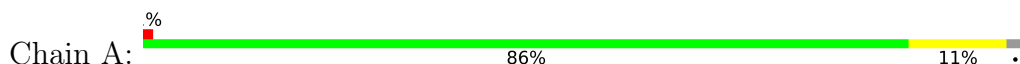
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	109	Total 109	O 109	0	0
3	F	87	Total 87	O 87	0	0
3	G	88	Total 88	O 88	0	0
3	H	114	Total 114	O 114	0	0

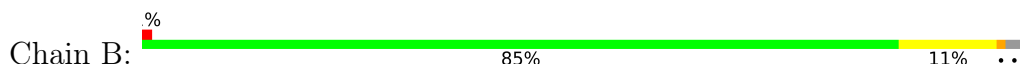
3 Residue-property plots [i](#)

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.

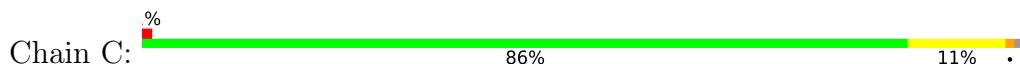
- Molecule 1: Transcriptional activator protein LasR



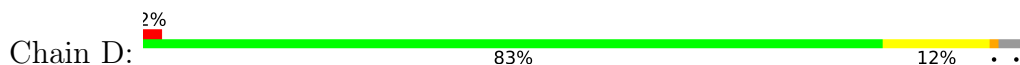
- Molecule 1: Transcriptional activator protein LasR



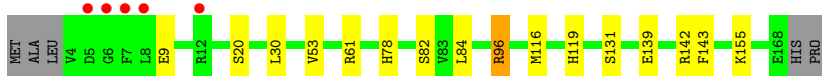
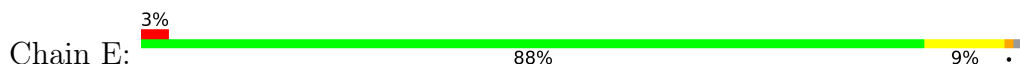
- Molecule 1: Transcriptional activator protein LasR



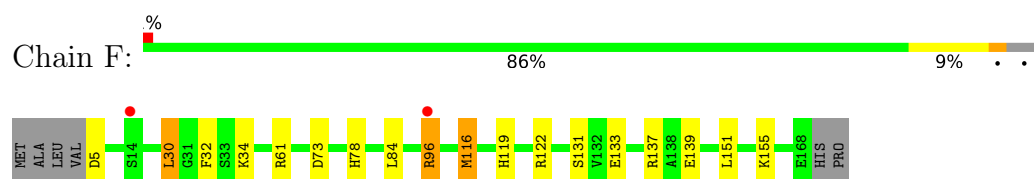
- Molecule 1: Transcriptional activator protein LasR



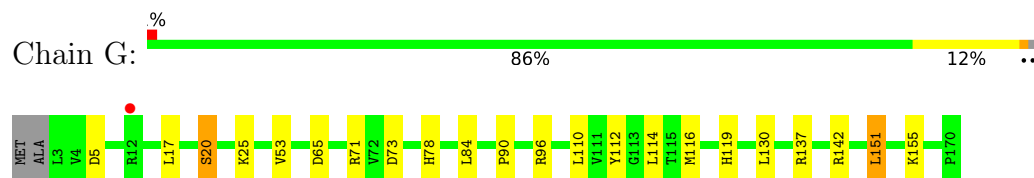
- Molecule 1: Transcriptional activator protein LasR



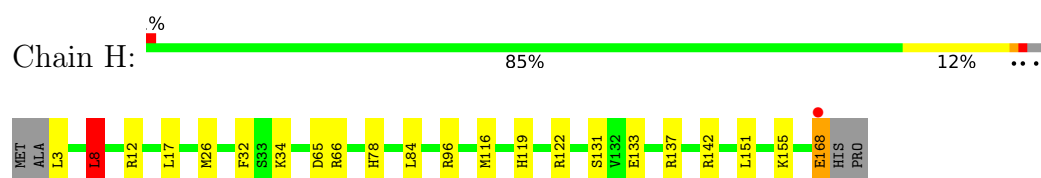
- Molecule 1: Transcriptional activator protein LasR



- Molecule 1: Transcriptional activator protein LasR



- Molecule 1: Transcriptional activator protein LasR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.28Å 84.47Å 156.20Å 90.00° 95.69° 90.00°	Depositor
Resolution (Å)	42.23 – 1.70 42.23 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (42.23-1.70) 95.0 (42.23-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.179 , 0.210 0.190 , 0.218	Depositor DCC
R_{free} test set	7321 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	14.0	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11472	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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 24.85 % 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 3.5434e-03. 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: FXS

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	1.00	0/1356	0.99	2/1837 (0.1%)
1	B	0.96	1/1356 (0.1%)	1.01	7/1837 (0.4%)
1	C	0.97	0/1344	0.98	5/1821 (0.3%)
1	D	0.97	0/1321	0.97	2/1789 (0.1%)
1	E	1.02	0/1348	1.01	3/1826 (0.2%)
1	F	1.00	1/1341 (0.1%)	1.01	5/1816 (0.3%)
1	G	0.99	0/1372	0.98	5/1860 (0.3%)
1	H	1.02	0/1344	1.10	12/1821 (0.7%)
All	All	0.99	2/10782 (0.0%)	1.01	41/14607 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	157	TYR	CE1-CZ	-5.42	1.31	1.38
1	F	139	GLU	CB-CG	-5.13	1.42	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	65	ASP	CB-CG-OD1	7.53	125.08	118.30
1	B	122	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	B	142	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	A	142	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	F	137	ARG	NE-CZ-NH1	-7.43	116.58	120.30
1	E	96	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	C	29	ASP	CB-CG-OD1	7.16	124.74	118.30
1	G	73	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	H	8	LEU	CB-CG-CD1	6.86	122.66	111.00
1	H	66	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	E	96	ARG	NE-CZ-NH2	-6.83	116.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	137	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	B	73	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	F	73	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	B	122	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	H	96	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	D	142	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	H	137	ARG	NE-CZ-NH1	-6.15	117.23	120.30
1	B	142	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	H	137	ARG	NE-CZ-NH2	6.09	123.35	120.30
1	B	73	ASP	CB-CG-OD1	6.08	123.78	118.30
1	G	65	ASP	CB-CG-OD1	6.08	123.78	118.30
1	C	61	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	H	122	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	H	122	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	C	26	MET	CG-SD-CE	-5.76	90.98	100.20
1	C	29	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	F	73	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	73	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	H	65	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	G	142	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	G	65	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	G	71	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	H	26	MET	CG-SD-CE	-5.18	91.91	100.20
1	H	116	MET	CG-SD-CE	5.17	108.48	100.20
1	B	116	MET	CG-SD-CE	5.15	108.44	100.20
1	E	142	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	F	30	LEU	CB-CG-CD2	5.11	119.68	111.00
1	C	142	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	H	142	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	A	122	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1312	0	1267	13	0
1	B	1312	0	1267	13	0
1	C	1310	0	1261	12	0
1	D	1287	0	1237	14	0
1	E	1304	0	1256	8	0
1	F	1297	0	1247	12	0
1	G	1326	0	1279	12	0
1	H	1310	0	1261	12	0
2	A	33	0	0	1	0
2	B	33	0	0	0	0
2	C	33	0	0	0	0
2	D	33	0	0	1	0
2	E	33	0	0	1	0
2	F	33	0	0	0	0
2	G	33	0	0	1	0
2	H	33	0	0	0	0
3	A	92	0	0	2	0
3	B	85	0	0	3	0
3	C	103	0	0	7	0
3	D	72	0	0	8	1
3	E	109	0	0	4	1
3	F	87	0	0	6	1
3	G	88	0	0	3	0
3	H	114	0	0	4	1
All	All	11472	0	10075	94	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 5.

All (94) 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:C:116:MET:HG3	3:C:472:HOH:O	1.38	1.22
1:F:61:ARG:NH1	3:F:401:HOH:O	2.06	0.88
1:H:3:LEU:N	3:H:401:HOH:O	2.10	0.84
1:C:3:LEU:N	3:C:401:HOH:O	2.10	0.84
1:F:122:ARG:NH1	3:F:402:HOH:O	2.14	0.79
1:C:78:HIS:HD2	3:C:497:HOH:O	1.66	0.77
1:C:151:LEU:HD22	3:C:472:HOH:O	1.87	0.74
1:D:122:ARG:CZ	3:D:403:HOH:O	2.36	0.74
1:A:103:GLU:OE2	3:A:401:HOH:O	2.08	0.72
1:H:32:PHE:CE2	1:H:151:LEU:HD21	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:HIS:HE1	1:E:84:LEU:O	1.75	0.69
1:G:78:HIS:HE1	1:G:84:LEU:O	1.75	0.69
1:H:8:LEU:O	1:H:12:ARG:HG2	1.93	0.69
1:F:96:ARG:N	1:F:96:ARG:HD3	2.08	0.69
1:D:72:VAL:HG23	3:D:410:HOH:O	1.95	0.67
1:F:5:ASP:N	3:F:403:HOH:O	2.27	0.66
1:A:61:ARG:CZ	3:A:409:HOH:O	2.44	0.66
1:C:78:HIS:HE1	1:C:84:LEU:O	1.80	0.65
1:D:110:LEU:HD13	2:D:300:FXS:O18	1.97	0.65
1:D:78:HIS:HE1	1:D:84:LEU:O	1.81	0.64
1:H:78:HIS:HE1	1:H:84:LEU:O	1.82	0.62
1:B:17:LEU:HD22	3:B:453:HOH:O	1.99	0.61
1:E:78:HIS:HD2	3:E:499:HOH:O	1.83	0.61
1:G:5:ASP:CB	3:G:475:HOH:O	2.47	0.61
1:A:32:PHE:CE2	1:A:151:LEU:HD21	2.36	0.61
1:C:94:GLN:HG2	3:C:435:HOH:O	2.01	0.60
1:F:96:ARG:CD	1:F:96:ARG:H	2.14	0.60
1:F:78:HIS:HE1	1:F:84:LEU:O	1.84	0.60
1:B:78:HIS:HE1	1:B:84:LEU:O	1.85	0.59
1:A:78:HIS:HE1	1:A:84:LEU:O	1.86	0.59
1:C:94:GLN:HG2	3:C:491:HOH:O	2.04	0.57
1:D:6:GLY:N	3:D:402:HOH:O	2.37	0.56
1:G:20[A]:SER:OG	1:G:53:VAL:HG13	2.04	0.56
1:D:122:ARG:NH2	3:D:403:HOH:O	2.39	0.56
1:G:110:LEU:HD13	2:G:300:FXS:O18	2.06	0.56
1:F:96:ARG:CD	1:F:96:ARG:N	2.68	0.55
2:E:300:FXS:O3	2:E:300:FXS:C21	2.55	0.54
1:E:139:GLU:HG2	1:E:143:PHE:CE2	2.44	0.53
1:F:34:LYS:HB2	1:F:131[A]:SER:OG	2.08	0.53
1:B:20[A]:SER:HB2	1:B:53:VAL:HG13	1.91	0.53
1:B:35:ILE:HG22	1:B:130:LEU:HD23	1.90	0.53
1:A:32:PHE:CZ	1:A:151:LEU:HD11	2.44	0.52
1:B:20[A]:SER:OG	1:B:24:GLN:NE2	2.42	0.52
1:H:168:GLU:HB3	3:H:435:HOH:O	2.09	0.52
1:H:119:HIS:HD2	3:H:445:HOH:O	1.92	0.52
1:G:119:HIS:HD2	3:G:432:HOH:O	1.92	0.52
1:H:34:LYS:HB2	1:H:131[A]:SER:OG	2.09	0.52
1:E:96:ARG:NH2	3:E:403:HOH:O	2.44	0.51
1:H:3:LEU:CA	3:H:401:HOH:O	2.57	0.50
1:D:14:SER:OG	3:D:401:HOH:O	2.09	0.50
1:F:119:HIS:HD2	3:F:437:HOH:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:32:PHE:CZ	1:H:151:LEU:HD11	2.47	0.50
1:G:116:MET:CE	3:G:412:HOH:O	2.60	0.50
1:E:20[A]:SER:OG	1:E:53:VAL:HG13	2.12	0.50
1:B:119:HIS:HD2	3:B:436:HOH:O	1.94	0.49
1:B:20[B]:SER:HB3	1:B:53:VAL:HG13	1.93	0.49
1:G:114:LEU:HD11	1:G:151:LEU:HD12	1.95	0.48
1:D:114:LEU:HD21	1:D:151:LEU:HD11	1.96	0.48
1:C:85:PRO:HB3	1:C:116:MET:SD	2.55	0.47
1:B:3:LEU:N	3:B:405:HOH:O	2.48	0.47
1:B:30:LEU:HD23	1:B:151:LEU:HD23	1.97	0.46
1:C:17:LEU:C	1:C:17:LEU:HD13	2.36	0.46
1:B:30:LEU:CD2	1:B:151:LEU:HD23	2.45	0.46
1:E:119:HIS:HD2	3:E:473:HOH:O	1.99	0.46
1:H:32:PHE:HZ	1:H:151:LEU:HD11	1.80	0.46
1:C:48:GLU:CD	1:C:48:GLU:H	2.18	0.46
1:A:85:PRO:HB3	1:A:116:MET:SD	2.55	0.46
1:D:61:ARG:CZ	3:D:408:HOH:O	2.63	0.46
1:A:24:GLN:HE21	1:A:54:GLY:HA2	1.81	0.46
1:C:119:HIS:HD2	3:C:444:HOH:O	1.99	0.45
1:F:116:MET:CE	3:F:407:HOH:O	2.65	0.45
1:B:139:GLU:HA	1:B:142:ARG:NH1	2.33	0.44
1:C:20[A]:SER:OG	1:C:53:VAL:HG13	2.18	0.43
1:D:8:LEU:HD12	1:D:8:LEU:HA	1.84	0.43
1:B:17:LEU:HD13	1:B:17:LEU:C	2.39	0.43
1:D:85:PRO:HB3	1:D:116:MET:SD	2.58	0.43
1:B:16:LYS:O	1:B:20[B]:SER:OG	2.33	0.43
1:E:61:ARG:CZ	3:E:416:HOH:O	2.67	0.43
1:E:82:SER:O	1:E:119:HIS:HE1	2.02	0.42
2:A:300:FXS:C21	2:A:300:FXS:O3	2.67	0.42
1:D:119:HIS:HD2	3:D:426:HOH:O	2.02	0.42
1:D:61:ARG:NH1	3:D:408:HOH:O	2.52	0.42
1:G:17:LEU:C	1:G:17:LEU:HD13	2.40	0.41
1:H:17:LEU:C	1:H:17:LEU:HD13	2.40	0.41
1:D:111:VAL:HG13	1:D:112:TYR:N	2.36	0.41
1:A:89:GLU:OE2	1:A:137:ARG:HD3	2.20	0.41
1:F:116:MET:HE2	3:F:407:HOH:O	2.19	0.41
1:A:135:GLU:OE1	1:G:137:ARG:NH2	2.53	0.41
1:A:20[A]:SER:OG	1:A:24:GLN:NE2	2.53	0.41
1:A:103:GLU:HG3	1:G:96:ARG:NE	2.36	0.41
1:F:32:PHE:CZ	1:F:151:LEU:HD11	2.56	0.41
1:A:135:GLU:HG3	1:G:112:TYR:OH	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLU:HG3	1:G:96:ARG:HE	1.86	0.41
1:H:32:PHE:HE2	1:H:151:LEU:HD21	1.78	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:E:476:HOH:O	3:H:454:HOH:O[1_655]	2.09	0.11
3:D:437:HOH:O	3:F:464:HOH:O[2_756]	2.19	0.01

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	166/170 (98%)	163 (98%)	3 (2%)	0	100	100
1	B	166/170 (98%)	165 (99%)	1 (1%)	0	100	100
1	C	164/170 (96%)	164 (100%)	0	0	100	100
1	D	161/170 (95%)	160 (99%)	1 (1%)	0	100	100
1	E	165/170 (97%)	164 (99%)	1 (1%)	0	100	100
1	F	164/170 (96%)	163 (99%)	1 (1%)	0	100	100
1	G	168/170 (99%)	166 (99%)	2 (1%)	0	100	100
1	H	164/170 (96%)	162 (99%)	2 (1%)	0	100	100
All	All	1318/1360 (97%)	1307 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	137/138 (99%)	134 (98%)	3 (2%)	55	36
1	B	137/138 (99%)	134 (98%)	3 (2%)	55	36
1	C	135/138 (98%)	129 (96%)	6 (4%)	31	12
1	D	132/138 (96%)	126 (96%)	6 (4%)	30	11
1	E	136/138 (99%)	130 (96%)	6 (4%)	31	12
1	F	135/138 (98%)	130 (96%)	5 (4%)	37	16
1	G	138/138 (100%)	131 (95%)	7 (5%)	26	9
1	H	135/138 (98%)	131 (97%)	4 (3%)	44	24
All	All	1085/1104 (98%)	1045 (96%)	40 (4%)	39	16

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	48	GLU
1	A	155	LYS
1	B	8	LEU
1	B	130	LEU
1	B	155	LYS
1	C	3	LEU
1	C	12	ARG
1	C	66	ARG
1	C	133	GLU
1	C	151	LEU
1	C	155	LYS
1	D	8	LEU
1	D	48	GLU
1	D	106	SER
1	D	133	GLU
1	D	151	LEU
1	D	155	LYS
1	E	9	GLU

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Mol	Chain	Res	Type
1	E	30	LEU
1	E	116	MET
1	E	131[A]	SER
1	E	131[B]	SER
1	E	155	LYS
1	F	30	LEU
1	F	96	ARG
1	F	116	MET
1	F	133	GLU
1	F	155	LYS
1	G	20[A]	SER
1	G	20[B]	SER
1	G	25	LYS
1	G	90	PRO
1	G	130	LEU
1	G	151	LEU
1	G	155	LYS
1	H	8	LEU
1	H	133	GLU
1	H	155	LYS
1	H	168	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	49	ASN
1	A	78	HIS
1	A	119	HIS
1	B	24	GLN
1	B	78	HIS
1	C	78	HIS
1	C	119	HIS
1	D	45	GLN
1	D	78	HIS
1	E	63	HIS
1	E	78	HIS
1	E	94	GLN
1	E	119	HIS
1	F	49	ASN
1	F	78	HIS
1	F	119	HIS

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Mol	Chain	Res	Type
1	G	78	HIS
1	G	119	HIS
1	H	45	GLN
1	H	78	HIS
1	H	119	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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	FXS	A	300	-	33,35,35	2.17	8 (24%)	41,49,49	1.66	12 (29%)
2	FXS	B	300	-	33,35,35	2.16	5 (15%)	41,49,49	1.24	5 (12%)
2	FXS	C	300	-	33,35,35	2.27	9 (27%)	41,49,49	1.47	8 (19%)
2	FXS	D	300	-	33,35,35	2.43	6 (18%)	41,49,49	2.00	15 (36%)
2	FXS	E	300	-	33,35,35	2.27	6 (18%)	41,49,49	1.71	12 (29%)
2	FXS	F	300	-	33,35,35	2.31	4 (12%)	41,49,49	2.00	11 (26%)
2	FXS	G	300	-	33,35,35	2.19	7 (21%)	41,49,49	1.82	15 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FXS	H	300	-	33,35,35	2.01	9 (27%)	41,49,49	1.99	14 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FXS	A	300	-	-	0/21/25/25	0/3/3/3
2	FXS	B	300	-	-	0/21/25/25	0/3/3/3
2	FXS	C	300	-	-	0/21/25/25	0/3/3/3
2	FXS	D	300	-	-	0/21/25/25	0/3/3/3
2	FXS	E	300	-	-	0/21/25/25	0/3/3/3
2	FXS	F	300	-	-	0/21/25/25	0/3/3/3
2	FXS	G	300	-	-	0/21/25/25	0/3/3/3
2	FXS	H	300	-	-	0/21/25/25	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	300	FXS	C26-N1	-3.97	1.38	1.45
2	A	300	FXS	C26-N1	-3.82	1.38	1.45
2	E	300	FXS	C26-N1	-3.30	1.39	1.45
2	G	300	FXS	C15-N16	-3.09	1.40	1.45
2	B	300	FXS	C15-N16	-3.07	1.40	1.45
2	A	300	FXS	C15-N16	-3.05	1.40	1.45
2	B	300	FXS	C26-N1	-3.04	1.40	1.45
2	D	300	FXS	C26-N1	-2.92	1.40	1.45
2	C	300	FXS	C26-N1	-2.79	1.40	1.45
2	H	300	FXS	C26-N1	-2.79	1.40	1.45
2	C	300	FXS	C15-N16	-2.73	1.40	1.45
2	D	300	FXS	C15-N16	-2.65	1.40	1.45
2	E	300	FXS	O20-C1	-2.64	1.36	1.40
2	G	300	FXS	C26-N1	-2.60	1.40	1.45
2	C	300	FXS	C14-C15	-2.43	1.34	1.39
2	F	300	FXS	C25-C26	-2.33	1.35	1.41
2	G	300	FXS	O20-C1	-2.28	1.36	1.40
2	E	300	FXS	C15-N16	-2.20	1.41	1.45
2	H	300	FXS	O20-C1	-2.18	1.36	1.40
2	G	300	FXS	C10-C15	-2.13	1.36	1.41
2	H	300	FXS	C15-N16	-2.13	1.41	1.45
2	C	300	FXS	C10-C15	-2.08	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	300	FXS	C9-N8	-2.04	1.29	1.33
2	A	300	FXS	C14-C15	-2.01	1.35	1.39
2	H	300	FXS	C12-C11	2.10	1.43	1.38
2	H	300	FXS	O17-C9	2.13	1.27	1.23
2	B	300	FXS	O20-C21	2.22	1.43	1.35
2	E	300	FXS	O20-C21	2.28	1.43	1.35
2	H	300	FXS	C11-C10	2.33	1.43	1.39
2	A	300	FXS	O20-C21	2.33	1.43	1.35
2	G	300	FXS	O20-C21	2.37	1.43	1.35
2	C	300	FXS	C11-C10	2.51	1.43	1.39
2	C	300	FXS	O20-C21	2.60	1.44	1.35
2	A	300	FXS	O17-C9	2.61	1.28	1.23
2	D	300	FXS	O17-C9	2.71	1.28	1.23
2	A	300	FXS	C11-C10	2.72	1.44	1.39
2	D	300	FXS	O20-C21	2.84	1.45	1.35
2	C	300	FXS	O17-C9	3.63	1.30	1.23
2	C	300	FXS	O19-N16	3.85	1.29	1.22
2	B	300	FXS	O19-N16	5.01	1.31	1.22
2	H	300	FXS	O19-N16	5.54	1.32	1.22
2	A	300	FXS	O19-N16	5.90	1.33	1.22
2	G	300	FXS	O19-N16	6.22	1.33	1.22
2	H	300	FXS	O3-N1	6.72	1.34	1.22
2	E	300	FXS	O19-N16	7.05	1.35	1.22
2	A	300	FXS	O3-N1	7.37	1.36	1.22
2	F	300	FXS	O19-N16	7.50	1.36	1.22
2	G	300	FXS	O3-N1	8.03	1.37	1.22
2	F	300	FXS	O3-N1	8.24	1.37	1.22
2	D	300	FXS	O19-N16	8.35	1.37	1.22
2	E	300	FXS	O3-N1	8.45	1.37	1.22
2	D	300	FXS	O3-N1	8.45	1.37	1.22
2	B	300	FXS	O3-N1	8.83	1.38	1.22
2	C	300	FXS	O3-N1	9.25	1.39	1.22

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	300	FXS	O17-C9-C10	-5.05	111.57	120.98
2	D	300	FXS	C12-C13-C14	-4.53	113.99	120.20
2	F	300	FXS	O20-C21-O22	-4.05	114.22	123.10
2	H	300	FXS	O17-C9-C10	-3.66	114.17	120.98
2	A	300	FXS	O17-C9-C10	-3.63	114.22	120.98
2	G	300	FXS	O17-C9-C10	-3.53	114.40	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	300	FXS	C12-C13-C14	-3.39	115.55	120.20
2	F	300	FXS	C3-C2-C1	-3.32	116.40	122.54
2	D	300	FXS	C11-C10-C15	-3.22	113.96	118.35
2	H	300	FXS	C3-C2-C1	-3.11	116.77	122.54
2	E	300	FXS	C3-C2-C1	-3.04	116.92	122.54
2	D	300	FXS	BR2-C4-C5	-3.02	115.06	119.27
2	E	300	FXS	C12-C13-C14	-2.77	116.41	120.20
2	H	300	FXS	C6-C5-C4	-2.74	115.61	119.94
2	G	300	FXS	C11-C10-C15	-2.67	114.71	118.35
2	E	300	FXS	O17-C9-C10	-2.56	116.21	120.98
2	H	300	FXS	C30-C25-C21	-2.49	113.55	118.67
2	H	300	FXS	BR2-C4-C5	-2.49	115.79	119.27
2	B	300	FXS	O17-C9-C10	-2.48	116.36	120.98
2	G	300	FXS	C3-C2-C1	-2.45	118.00	122.54
2	E	300	FXS	C30-C25-C21	-2.32	113.91	118.67
2	C	300	FXS	O17-C9-C10	-2.31	116.68	120.98
2	A	300	FXS	O20-C21-O22	-2.27	118.11	123.10
2	C	300	FXS	C30-C25-C21	-2.25	114.04	118.67
2	H	300	FXS	O20-C21-O22	-2.25	118.16	123.10
2	G	300	FXS	BR2-C4-C5	-2.15	116.27	119.27
2	F	300	FXS	C12-C13-C14	-2.11	117.30	120.20
2	D	300	FXS	C3-C2-C1	-2.04	118.77	122.54
2	E	300	FXS	C30-C25-C26	2.00	121.09	118.35
2	A	300	FXS	BR1-C2-C1	2.01	121.49	118.54
2	A	300	FXS	C13-C14-C15	2.01	122.07	118.64
2	D	300	FXS	BR1-C2-C1	2.03	121.51	118.54
2	E	300	FXS	C4-C3-C2	2.05	121.54	118.85
2	G	300	FXS	O20-C21-C25	2.07	116.97	111.81
2	G	300	FXS	C15-C10-C9	2.07	128.40	123.49
2	C	300	FXS	C30-C25-C26	2.08	121.19	118.35
2	E	300	FXS	C13-C14-C15	2.10	122.23	118.64
2	A	300	FXS	C6-C1-C2	2.13	119.89	116.95
2	E	300	FXS	C27-C26-N1	2.18	119.04	116.50
2	D	300	FXS	C15-C10-C9	2.25	128.83	123.49
2	D	300	FXS	O20-C21-C25	2.28	117.52	111.81
2	B	300	FXS	O20-C21-C25	2.30	117.56	111.81
2	C	300	FXS	C10-C9-N8	2.33	121.95	117.42
2	G	300	FXS	C1-O20-C21	2.33	123.42	117.48
2	G	300	FXS	C14-C15-C10	2.34	122.88	119.34
2	A	300	FXS	C30-C25-C26	2.34	121.55	118.35
2	A	300	FXS	C7-N8-C9	2.38	127.70	121.83
2	H	300	FXS	O3-N1-C26	2.39	123.21	118.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	FXS	C29-C28-C27	2.41	123.50	120.20
2	A	300	FXS	O20-C21-C25	2.43	117.89	111.81
2	G	300	FXS	O20-C1-C6	2.44	122.47	118.44
2	F	300	FXS	C13-C12-C11	2.46	123.57	120.20
2	B	300	FXS	C7-N8-C9	2.49	127.97	121.83
2	C	300	FXS	C1-O20-C21	2.50	123.87	117.48
2	F	300	FXS	O20-C21-C25	2.51	118.08	111.81
2	F	300	FXS	BR1-C2-C3	2.54	122.72	118.39
2	C	300	FXS	BR1-C2-C1	2.59	122.34	118.54
2	D	300	FXS	C6-C1-C2	2.60	120.53	116.95
2	D	300	FXS	BR2-C4-C3	2.61	122.91	119.27
2	D	300	FXS	C13-C14-C15	2.65	123.15	118.64
2	A	300	FXS	C14-C15-N16	2.67	119.61	116.50
2	G	300	FXS	C30-C25-C26	2.68	122.00	118.35
2	H	300	FXS	C7-N8-C9	2.69	128.47	121.83
2	D	300	FXS	C12-C11-C10	2.69	124.93	119.82
2	D	300	FXS	C1-O20-C21	2.71	124.39	117.48
2	B	300	FXS	C1-O20-C21	2.71	124.41	117.48
2	E	300	FXS	O20-C21-C25	2.73	118.64	111.81
2	G	300	FXS	BR1-C2-C1	2.76	122.59	118.54
2	H	300	FXS	O20-C21-C25	2.77	118.72	111.81
2	E	300	FXS	BR1-C2-C1	2.77	122.61	118.54
2	H	300	FXS	O20-C1-C6	2.80	123.06	118.44
2	E	300	FXS	C6-C1-C2	2.83	120.85	116.95
2	H	300	FXS	C30-C25-C26	2.87	122.27	118.35
2	D	300	FXS	C10-C9-N8	2.89	123.05	117.42
2	D	300	FXS	C14-C15-N16	2.97	119.96	116.50
2	F	300	FXS	C6-C1-C2	3.01	121.11	116.95
2	B	300	FXS	C6-C1-C2	3.04	121.14	116.95
2	C	300	FXS	O20-C21-C25	3.05	119.43	111.81
2	G	300	FXS	C7-N8-C9	3.05	129.37	121.83
2	A	300	FXS	C10-C9-N8	3.19	123.65	117.42
2	G	300	FXS	C10-C9-N8	3.21	123.68	117.42
2	G	300	FXS	C6-C1-C2	3.35	121.57	116.95
2	F	300	FXS	C4-C3-C2	3.43	123.36	118.85
2	F	300	FXS	O20-C1-C6	3.55	124.30	118.44
2	F	300	FXS	C10-C9-N8	3.62	124.47	117.42
2	H	300	FXS	C6-C1-C2	3.62	121.94	116.95
2	H	300	FXS	C10-C9-N8	3.66	124.56	117.42
2	C	300	FXS	C6-C1-C2	3.68	122.02	116.95
2	E	300	FXS	C7-N8-C9	3.76	131.11	121.83
2	H	300	FXS	BR1-C2-C1	4.01	124.42	118.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	FXS	O20-C1-C6	4.05	125.13	118.44
2	D	300	FXS	C7-N8-C9	4.25	132.32	121.83

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
2	A	300	FXS	1	0
2	D	300	FXS	1	0
2	E	300	FXS	1	0
2	G	300	FXS	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	166/170 (97%)	-0.19	1 (0%)	89 91	7, 15, 31, 45	0
1	B	166/170 (97%)	-0.22	1 (0%)	89 91	7, 15, 34, 45	0
1	C	166/170 (97%)	-0.17	2 (1%)	79 83	7, 14, 32, 64	0
1	D	163/170 (95%)	-0.05	4 (2%)	57 62	8, 17, 36, 64	0
1	E	165/170 (97%)	-0.08	5 (3%)	50 55	6, 14, 34, 57	0
1	F	164/170 (96%)	-0.01	2 (1%)	79 83	8, 15, 35, 50	0
1	G	168/170 (98%)	-0.12	1 (0%)	89 91	7, 15, 32, 44	0
1	H	166/170 (97%)	-0.23	1 (0%)	89 91	5, 12, 27, 62	0
All	All	1324/1360 (97%)	-0.13	17 (1%)	77 81	5, 15, 34, 64	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	96	ARG	4.5
1	E	7	PHE	3.6
1	H	168	GLU	3.6
1	E	12	ARG	3.2
1	E	8	LEU	3.1
1	E	6	GLY	3.0
1	D	7	PHE	2.9
1	C	168	GLU	2.8
1	D	168	GLU	2.8
1	G	12	ARG	2.6
1	D	6	GLY	2.5
1	F	14	SER	2.4
1	C	48	GLU	2.4
1	A	4	VAL	2.3
1	D	12	ARG	2.3
1	B	8	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	5	ASP	2.1

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. 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	B-factors(Å ²)	Q<0.9
2	FXS	E	300	33/33	0.98	0.08	12,15,24,33	0
2	FXS	G	300	33/33	0.98	0.08	12,15,25,33	0
2	FXS	A	300	33/33	0.98	0.09	11,14,26,34	0
2	FXS	C	300	33/33	0.98	0.11	11,15,28,34	0
2	FXS	H	300	33/33	0.98	0.08	9,13,22,31	0
2	FXS	D	300	33/33	0.98	0.09	13,18,33,40	0
2	FXS	B	300	33/33	0.98	0.09	10,15,26,33	0
2	FXS	F	300	33/33	0.99	0.07	12,16,26,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.