



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:38 AM GMT

PDB ID : 3FG8
Title : Crystal structure of PAS domain of RHA05790
Authors : Chang, C.; Xu, X.; Cui, H.; Savchenko, A.; Edwards, A.; Joachimiak, A.;
Midwest Center for Structural Genomics (MCSG)
Deposited on : 2008-12-05
Resolution : 1.80 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

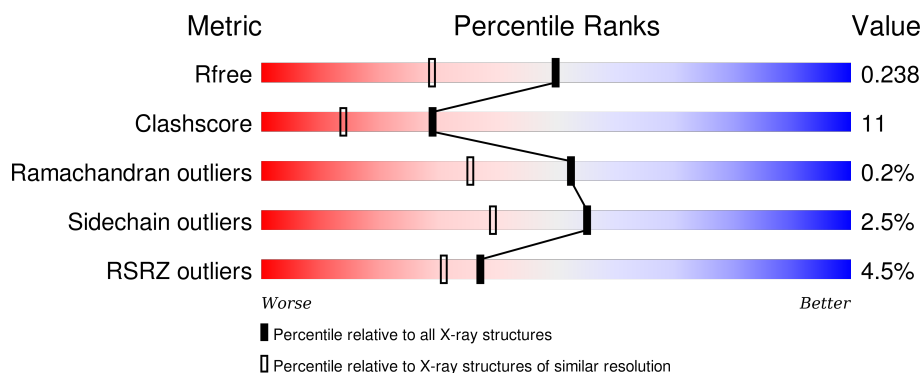
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	118	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>10%</div> </div> </div>
1	B	118	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	118	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	118	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div>•</div> <div>10%</div> </div> </div>
1	E	118	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>15%</div> <div>• •</div> <div>11%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	118	

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	3PB	A	301	-	-	-	X
2	3PB	B	301	-	-	-	X
2	3PB	C	301	-	-	-	X
2	3PB	D	301	-	-	-	X
2	3PB	E	301	-	-	-	X
2	3PB	F	301	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6366 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 uncharacterized protein RHA05790.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	Se	0	15	0
			950	588	181	177	2	2			
1	B	105	Total	C	N	O	S	Se	0	10	0
			881	548	161	167	3	2			
1	C	105	Total	C	N	O	S	Se	0	12	0
			900	562	170	164	2	2			
1	D	106	Total	C	N	O	S	Se	0	16	0
			974	601	193	176	2	2			
1	E	105	Total	C	N	O	S	Se	0	12	0
			907	561	174	168	2	2			
1	F	105	Total	C	N	O	S	Se	0	11	0
			916	564	179	168	3	2			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	MSE	-	expression tag	UNP Q0S7I6
A	108	GLY	-	expression tag	UNP Q0S7I6
A	109	SER	-	expression tag	UNP Q0S7I6
A	110	SER	-	expression tag	UNP Q0S7I6
A	111	HIS	-	expression tag	UNP Q0S7I6
A	112	HIS	-	expression tag	UNP Q0S7I6
A	113	HIS	-	expression tag	UNP Q0S7I6
A	114	HIS	-	expression tag	UNP Q0S7I6
A	115	HIS	-	expression tag	UNP Q0S7I6
A	116	HIS	-	expression tag	UNP Q0S7I6
A	117	SER	-	expression tag	UNP Q0S7I6
A	118	SER	-	expression tag	UNP Q0S7I6
A	119	GLY	-	expression tag	UNP Q0S7I6
A	120	ARG	-	expression tag	UNP Q0S7I6
A	121	GLU	-	expression tag	UNP Q0S7I6
A	122	ASN	-	expression tag	UNP Q0S7I6
A	123	LEU	-	expression tag	UNP Q0S7I6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	TYR	-	expression tag	UNP Q0S7I6
A	125	PHE	-	expression tag	UNP Q0S7I6
A	126	GLN	-	expression tag	UNP Q0S7I6
A	127	GLY	-	expression tag	UNP Q0S7I6
B	107	MSE	-	expression tag	UNP Q0S7I6
B	108	GLY	-	expression tag	UNP Q0S7I6
B	109	SER	-	expression tag	UNP Q0S7I6
B	110	SER	-	expression tag	UNP Q0S7I6
B	111	HIS	-	expression tag	UNP Q0S7I6
B	112	HIS	-	expression tag	UNP Q0S7I6
B	113	HIS	-	expression tag	UNP Q0S7I6
B	114	HIS	-	expression tag	UNP Q0S7I6
B	115	HIS	-	expression tag	UNP Q0S7I6
B	116	HIS	-	expression tag	UNP Q0S7I6
B	117	SER	-	expression tag	UNP Q0S7I6
B	118	SER	-	expression tag	UNP Q0S7I6
B	119	GLY	-	expression tag	UNP Q0S7I6
B	120	ARG	-	expression tag	UNP Q0S7I6
B	121	GLU	-	expression tag	UNP Q0S7I6
B	122	ASN	-	expression tag	UNP Q0S7I6
B	123	LEU	-	expression tag	UNP Q0S7I6
B	124	TYR	-	expression tag	UNP Q0S7I6
B	125	PHE	-	expression tag	UNP Q0S7I6
B	126	GLN	-	expression tag	UNP Q0S7I6
B	127	GLY	-	expression tag	UNP Q0S7I6
C	107	MSE	-	expression tag	UNP Q0S7I6
C	108	GLY	-	expression tag	UNP Q0S7I6
C	109	SER	-	expression tag	UNP Q0S7I6
C	110	SER	-	expression tag	UNP Q0S7I6
C	111	HIS	-	expression tag	UNP Q0S7I6
C	112	HIS	-	expression tag	UNP Q0S7I6
C	113	HIS	-	expression tag	UNP Q0S7I6
C	114	HIS	-	expression tag	UNP Q0S7I6
C	115	HIS	-	expression tag	UNP Q0S7I6
C	116	HIS	-	expression tag	UNP Q0S7I6
C	117	SER	-	expression tag	UNP Q0S7I6
C	118	SER	-	expression tag	UNP Q0S7I6
C	119	GLY	-	expression tag	UNP Q0S7I6
C	120	ARG	-	expression tag	UNP Q0S7I6
C	121	GLU	-	expression tag	UNP Q0S7I6
C	122	ASN	-	expression tag	UNP Q0S7I6
C	123	LEU	-	expression tag	UNP Q0S7I6

Continued on next page...

Continued from previous page...

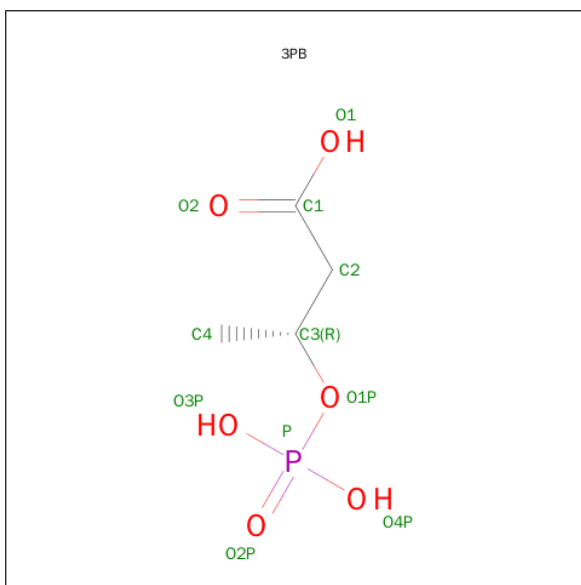
Chain	Residue	Modelled	Actual	Comment	Reference
C	124	TYR	-	expression tag	UNP Q0S7I6
C	125	PHE	-	expression tag	UNP Q0S7I6
C	126	GLN	-	expression tag	UNP Q0S7I6
C	127	GLY	-	expression tag	UNP Q0S7I6
D	107	MSE	-	expression tag	UNP Q0S7I6
D	108	GLY	-	expression tag	UNP Q0S7I6
D	109	SER	-	expression tag	UNP Q0S7I6
D	110	SER	-	expression tag	UNP Q0S7I6
D	111	HIS	-	expression tag	UNP Q0S7I6
D	112	HIS	-	expression tag	UNP Q0S7I6
D	113	HIS	-	expression tag	UNP Q0S7I6
D	114	HIS	-	expression tag	UNP Q0S7I6
D	115	HIS	-	expression tag	UNP Q0S7I6
D	116	HIS	-	expression tag	UNP Q0S7I6
D	117	SER	-	expression tag	UNP Q0S7I6
D	118	SER	-	expression tag	UNP Q0S7I6
D	119	GLY	-	expression tag	UNP Q0S7I6
D	120	ARG	-	expression tag	UNP Q0S7I6
D	121	GLU	-	expression tag	UNP Q0S7I6
D	122	ASN	-	expression tag	UNP Q0S7I6
D	123	LEU	-	expression tag	UNP Q0S7I6
D	124	TYR	-	expression tag	UNP Q0S7I6
D	125	PHE	-	expression tag	UNP Q0S7I6
D	126	GLN	-	expression tag	UNP Q0S7I6
D	127	GLY	-	expression tag	UNP Q0S7I6
E	107	MSE	-	expression tag	UNP Q0S7I6
E	108	GLY	-	expression tag	UNP Q0S7I6
E	109	SER	-	expression tag	UNP Q0S7I6
E	110	SER	-	expression tag	UNP Q0S7I6
E	111	HIS	-	expression tag	UNP Q0S7I6
E	112	HIS	-	expression tag	UNP Q0S7I6
E	113	HIS	-	expression tag	UNP Q0S7I6
E	114	HIS	-	expression tag	UNP Q0S7I6
E	115	HIS	-	expression tag	UNP Q0S7I6
E	116	HIS	-	expression tag	UNP Q0S7I6
E	117	SER	-	expression tag	UNP Q0S7I6
E	118	SER	-	expression tag	UNP Q0S7I6
E	119	GLY	-	expression tag	UNP Q0S7I6
E	120	ARG	-	expression tag	UNP Q0S7I6
E	121	GLU	-	expression tag	UNP Q0S7I6
E	122	ASN	-	expression tag	UNP Q0S7I6
E	123	LEU	-	expression tag	UNP Q0S7I6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	124	TYR	-	expression tag	UNP Q0S7I6
E	125	PHE	-	expression tag	UNP Q0S7I6
E	126	GLN	-	expression tag	UNP Q0S7I6
E	127	GLY	-	expression tag	UNP Q0S7I6
F	107	MSE	-	expression tag	UNP Q0S7I6
F	108	GLY	-	expression tag	UNP Q0S7I6
F	109	SER	-	expression tag	UNP Q0S7I6
F	110	SER	-	expression tag	UNP Q0S7I6
F	111	HIS	-	expression tag	UNP Q0S7I6
F	112	HIS	-	expression tag	UNP Q0S7I6
F	113	HIS	-	expression tag	UNP Q0S7I6
F	114	HIS	-	expression tag	UNP Q0S7I6
F	115	HIS	-	expression tag	UNP Q0S7I6
F	116	HIS	-	expression tag	UNP Q0S7I6
F	117	SER	-	expression tag	UNP Q0S7I6
F	118	SER	-	expression tag	UNP Q0S7I6
F	119	GLY	-	expression tag	UNP Q0S7I6
F	120	ARG	-	expression tag	UNP Q0S7I6
F	121	GLU	-	expression tag	UNP Q0S7I6
F	122	ASN	-	expression tag	UNP Q0S7I6
F	123	LEU	-	expression tag	UNP Q0S7I6
F	124	TYR	-	expression tag	UNP Q0S7I6
F	125	PHE	-	expression tag	UNP Q0S7I6
F	126	GLN	-	expression tag	UNP Q0S7I6
F	127	GLY	-	expression tag	UNP Q0S7I6

- Molecule 2 is (3R)-3-(PHOSPHONOOXY)BUTANOIC ACID (three-letter code: 3PB) (formula: C₄H₉O₆P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			11	4	6	1		
2	B	1	Total	C	O	P	0	0
			11	4	6	1		
2	C	1	Total	C	O	P	0	0
			11	4	6	1		
2	D	1	Total	C	O	P	0	0
			11	4	6	1		
2	E	1	Total	C	O	P	0	0
			11	4	6	1		
2	F	1	Total	C	O	P	0	0
			11	4	6	1		

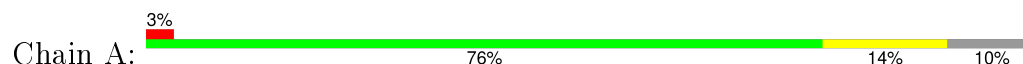
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	125	Total	O	0	0
			125	125		
3	B	129	Total	O	0	0
			129	129		
3	C	139	Total	O	0	0
			139	139		
3	D	130	Total	O	0	0
			130	130		
3	E	118	Total	O	0	0
			118	118		
3	F	131	Total	O	0	0
			131	131		

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.

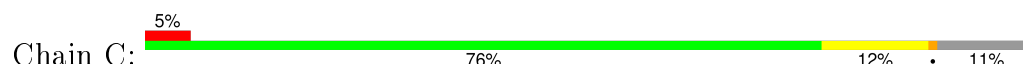
- Molecule 1: uncharacterized protein RHA05790



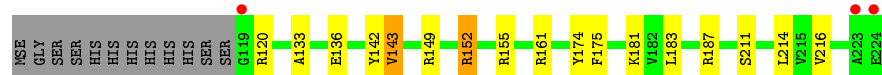
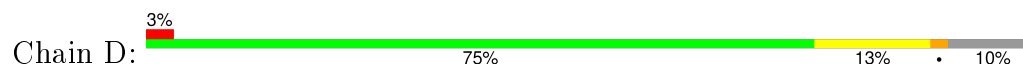
- Molecule 1: uncharacterized protein RHA05790



- Molecule 1: uncharacterized protein RHA05790



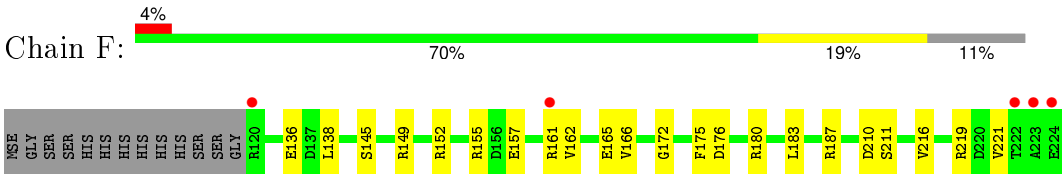
- Molecule 1: uncharacterized protein RHA05790



- Molecule 1: uncharacterized protein RHA05790



- Molecule 1: uncharacterized protein RHA05790



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.69 Å 55.89 Å 101.86 Å 90.00° 132.61° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 26.18 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-1.80) 99.3 (26.18-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 1.80 Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, R_{free}	0.168 , 0.223 0.183 , 0.238	Depositor DCC
R_{free} test set	2907 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.9	EDS
Estimated twinning fraction	0.049 for -h-2*k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 57284 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6366	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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 70.42 % 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 3.1340e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PB

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	0.73	0/977	0.81	0/1309
1	B	0.73	0/905	0.82	0/1217
1	C	0.70	0/939	0.83	1/1260 (0.1%)
1	D	0.68	0/998	0.74	0/1336
1	E	0.71	0/925	0.82	0/1242
1	F	0.68	0/931	0.78	0/1248
All	All	0.71	0/5675	0.80	1/7612 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	123	LEU	CA-CB-CG	5.12	127.08	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	119	GLY	Peptide

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	950	0	958	24	0
1	B	881	0	881	17	0
1	C	900	0	920	24	0
1	D	974	0	984	22	0
1	E	907	0	906	31	1
1	F	916	0	914	36	0
2	A	11	0	6	0	0
2	B	11	0	6	0	0
2	C	11	0	6	0	0
2	D	11	0	6	0	0
2	E	11	0	6	0	0
2	F	11	0	6	0	0
3	A	125	0	0	4	1
3	B	129	0	0	6	0
3	C	139	0	0	0	0
3	D	130	0	0	7	0
3	E	118	0	0	10	0
3	F	131	0	0	3	0
All	All	6366	0	5599	129	1

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 11.

All (129) 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:153[A]:ARG:NH1	1:F:187[A]:ARG:HH21	1.45	1.13
1:F:161[A]:ARG:HD3	1:F:166:VAL:HG11	1.21	1.12
1:C:153[A]:ARG:HH12	1:F:187[A]:ARG:NH2	1.48	1.10
1:E:149[B]:ARG:NH1	1:E:149[B]:ARG:HB2	1.64	1.10
1:F:161[A]:ARG:HD3	1:F:166:VAL:CG1	1.88	1.04
1:F:145[B]:SER:O	1:F:149[B]:ARG:HG2	1.60	1.00
1:D:136[B]:GLU:HG3	1:F:155[B]:ARG:CZ	1.94	0.98
1:A:154[B]:SER:OG	1:C:156[B]:ASP:OD2	1.84	0.95
1:D:149[B]:ARG:HH12	1:D:152[B]:ARG:HG2	1.30	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149[B]:ARG:HB2	1:E:149[B]:ARG:HH11	1.22	0.93
1:C:153[A]:ARG:HH12	1:F:187[A]:ARG:HH21	0.91	0.91
1:F:157:GLU:O	1:F:161[A]:ARG:HD2	1.69	0.91
1:F:161[A]:ARG:CD	1:F:166:VAL:HG11	2.02	0.89
1:D:120[A]:ARG:NH1	3:D:764:HOH:O	2.03	0.86
1:E:149[B]:ARG:CB	1:E:149[B]:ARG:HH11	1.91	0.84
1:E:171[A]:GLN:NE2	3:E:753:HOH:O	2.11	0.84
1:A:154[B]:SER:OG	1:C:156[B]:ASP:CG	2.17	0.82
1:A:154[B]:SER:OG	1:C:156[B]:ASP:OD1	1.98	0.81
1:B:202:THR:HG23	1:B:222:THR:HA	1.63	0.81
1:E:212[A]:GLY:HA3	3:E:727:HOH:O	1.81	0.79
1:C:120:ARG:N	1:C:120:ARG:HD2	1.98	0.78
1:A:211[B]:SER:O	1:A:211[B]:SER:OG	1.95	0.77
1:B:212[A]:GLY:HA2	3:B:359:HOH:O	1.84	0.77
3:B:623:HOH:O	1:F:136:GLU:HG3	1.82	0.77
1:C:153[A]:ARG:HH12	1:F:187[A]:ARG:CZ	1.99	0.76
1:F:149[B]:ARG:HB3	1:F:149[B]:ARG:NH1	2.02	0.75
1:D:120[B]:ARG:HG3	1:D:120[B]:ARG:HH11	1.54	0.72
1:D:136[B]:GLU:HG3	1:F:155[B]:ARG:NH2	2.06	0.71
1:B:162:VAL:O	1:B:165[A]:GLU:HG2	1.91	0.70
1:A:156[A]:ASP:OD1	3:A:248:HOH:O	2.08	0.70
1:A:135:ASP:OD2	1:A:139[A]:ARG:NH1	2.26	0.69
1:C:120:ARG:H	1:C:120:ARG:HD2	1.58	0.68
1:A:175:PHE:HE1	1:A:216[A]:VAL:HG11	1.57	0.67
1:A:198:SER:OG	1:E:139[A]:ARG:NH1	2.28	0.67
1:C:118:SER:CB	1:C:120:ARG:HH11	2.09	0.66
1:E:212[A]:GLY:O	3:E:233:HOH:O	2.13	0.66
1:D:136[B]:GLU:HG3	1:F:155[B]:ARG:NH1	2.11	0.65
1:B:211[A]:SER:OG	1:B:212[A]:GLY:N	2.30	0.63
1:A:152[A]:ARG:HD3	3:E:413:HOH:O	1.99	0.62
1:B:175:PHE:HE1	1:B:216:VAL:HG11	1.66	0.60
3:B:65:HOH:O	1:C:152:ARG:HD2	2.02	0.60
1:D:152[A]:ARG:NH2	3:D:366:HOH:O	2.35	0.59
1:D:120[B]:ARG:HG3	1:D:120[B]:ARG:NH1	2.17	0.59
1:F:187[B]:ARG:NH1	3:F:270:HOH:O	2.24	0.58
1:F:149[B]:ARG:HB3	1:F:149[B]:ARG:CZ	2.32	0.58
1:E:171[B]:GLN:NE2	3:E:695:HOH:O	2.36	0.58
1:E:143[B]:VAL:HG13	1:E:143[B]:VAL:O	2.04	0.57
1:C:153[A]:ARG:NH1	1:F:187[A]:ARG:NH2	2.22	0.56
1:D:136[B]:GLU:HA	1:D:136[B]:GLU:OE1	2.05	0.56
1:F:162:VAL:HB	1:F:165:GLU:HG3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152[A]:ARG:HH11	1:C:155:ARG:NH1	2.04	0.56
1:C:135:ASP:OD2	1:C:139[A]:ARG:NH1	2.38	0.56
1:D:136[B]:GLU:HG2	3:D:719:HOH:O	2.06	0.55
1:F:149[B]:ARG:NH2	3:F:383:HOH:O	2.40	0.55
1:C:153[A]:ARG:HH12	1:F:187[A]:ARG:NE	2.04	0.55
1:B:155[A]:ARG:CZ	1:B:159[A]:LEU:CD1	2.85	0.55
1:D:149[B]:ARG:NH1	3:D:633:HOH:O	2.40	0.54
1:A:175:PHE:CE1	1:A:216[A]:VAL:HG11	2.40	0.54
1:F:149[B]:ARG:CZ	1:F:149[B]:ARG:HA	2.38	0.54
1:A:152[A]:ARG:NH1	1:C:155:ARG:NH1	2.56	0.54
1:A:201:MSE:HE3	1:E:139[A]:ARG:HH12	1.74	0.53
1:D:149[B]:ARG:NH1	1:D:152[B]:ARG:HG2	2.12	0.53
1:F:149[B]:ARG:CZ	1:F:149[B]:ARG:CB	2.88	0.52
1:E:149[B]:ARG:NH1	1:E:149[B]:ARG:CB	2.52	0.52
1:E:139[A]:ARG:CZ	3:E:328:HOH:O	2.57	0.52
1:D:187[B]:ARG:HA	1:D:187[B]:ARG:NE	2.25	0.51
1:E:143[B]:VAL:CG1	1:E:143[B]:VAL:O	2.59	0.51
1:C:175:PHE:HE1	1:C:216[A]:VAL:HG11	1.74	0.51
1:D:133:ALA:HB3	1:D:142:TYR:HB3	1.93	0.51
1:D:175:PHE:HE1	1:D:216[A]:VAL:HG11	1.77	0.50
1:E:161[B]:ARG:HD2	1:E:166:VAL:HG11	1.92	0.49
1:A:133:ALA:HB3	1:A:142:TYR:HB3	1.94	0.49
1:B:155[B]:ARG:HD2	3:B:623:HOH:O	2.11	0.49
1:C:207:ALA:CB	1:C:216[B]:VAL:HG12	2.43	0.49
1:B:161:ARG:NH1	3:B:735:HOH:O	2.46	0.49
3:D:602:HOH:O	1:F:155[A]:ARG:HD3	2.14	0.48
1:D:120[B]:ARG:NH1	3:D:306:HOH:O	2.46	0.48
1:B:155[A]:ARG:CZ	1:B:159[A]:LEU:HD11	2.43	0.48
1:E:149[B]:ARG:CZ	1:E:149[B]:ARG:HB2	2.38	0.47
1:B:210:ASP:OD1	3:B:18:HOH:O	2.20	0.47
1:A:198:SER:OG	1:E:139[A]:ARG:CZ	2.62	0.47
1:F:157:GLU:O	1:F:161[A]:ARG:CD	2.54	0.47
1:C:176:ASP:OD1	1:C:180[A]:ARG:HD2	2.15	0.47
1:C:153[A]:ARG:NH1	1:F:187[A]:ARG:HE	2.13	0.47
1:A:181[B]:LYS:HA	1:A:181[B]:LYS:HD3	1.64	0.47
1:D:155[B]:ARG:NH1	3:D:98:HOH:O	2.46	0.46
1:E:139[A]:ARG:NH1	3:E:722:HOH:O	2.48	0.46
1:A:181[C]:LYS:HB2	1:A:181[C]:LYS:HE2	1.30	0.46
1:C:118:SER:CB	1:C:120:ARG:NH1	2.78	0.46
1:A:211[A]:SER:OG	3:A:448:HOH:O	2.15	0.46
1:D:183:LEU:HD21	1:D:214[A]:LEU:HD12	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155[A]:ARG:HG2	1:B:159[A]:LEU:HD12	1.97	0.45
1:E:175:PHE:HE1	1:E:216[A]:VAL:HG11	1.81	0.45
1:A:152[A]:ARG:NH1	1:C:155:ARG:HH12	2.14	0.45
1:A:152[A]:ARG:NH1	1:E:136:GLU:OE1	2.49	0.45
1:E:149[A]:ARG:HH12	1:E:152:ARG:CZ	2.30	0.45
1:F:149[B]:ARG:HB3	1:F:149[B]:ARG:HH11	1.81	0.45
1:F:175:PHE:HE1	1:F:216[A]:VAL:HG11	1.81	0.45
1:A:187[A]:ARG:HD2	1:A:187[A]:ARG:HA	1.84	0.44
1:D:181:LYS:HG2	1:F:211:SER:HB3	1.99	0.44
1:E:119:GLY:N	1:E:120:ARG:HG2	2.33	0.44
1:C:153[A]:ARG:HH12	1:F:187[A]:ARG:HE	1.64	0.44
1:F:176:ASP:OD1	1:F:180:ARG:HD3	2.17	0.44
1:B:182:VAL:HG11	1:B:214:LEU:HD13	2.00	0.44
1:E:139[B]:ARG:NH2	3:E:426:HOH:O	2.43	0.43
1:C:153[A]:ARG:HH22	1:F:187[A]:ARG:NE	2.17	0.43
1:E:143[B]:VAL:HG11	1:E:148:LEU:HD21	2.01	0.43
1:E:192[A]:ARG:HG3	3:E:509:HOH:O	2.18	0.43
1:B:123:LEU:HB2	1:F:180:ARG:HG2	2.00	0.43
1:A:198:SER:OG	1:E:139[A]:ARG:NH2	2.51	0.43
1:B:159[B]:LEU:HD12	1:B:159[B]:LEU:HA	1.82	0.42
1:F:172:GLY:HA2	3:F:547:HOH:O	2.19	0.42
1:E:164:THR:HG23	3:E:387:HOH:O	2.20	0.42
1:A:153[B]:ARG:NH2	3:A:471:HOH:O	2.44	0.42
1:E:149[B]:ARG:CA	1:E:149[B]:ARG:HH11	2.31	0.42
1:E:174:TYR:CD1	1:E:174:TYR:C	2.93	0.42
1:E:133:ALA:HB3	1:E:142:TYR:HB3	2.03	0.41
1:B:135:ASP:HB3	1:B:141:ILE:HD13	2.02	0.41
1:F:210:ASP:OD1	1:F:211:SER:OG	2.28	0.41
1:D:174:TYR:CD1	1:D:174:TYR:C	2.93	0.41
1:F:138:LEU:HD21	1:F:183:LEU:HD11	2.02	0.41
1:B:155[A]:ARG:NE	1:B:159[A]:LEU:HD11	2.36	0.41
1:D:143[B]:VAL:HG13	1:D:143[B]:VAL:O	2.20	0.41
1:A:152[A]:ARG:HG2	3:A:304:HOH:O	2.20	0.41
1:F:219:ARG:NH1	1:F:221:VAL:HG12	2.35	0.41
1:E:149[A]:ARG:O	1:E:149[A]:ARG:NH1	2.46	0.41
1:D:149[B]:ARG:HA	1:D:149[B]:ARG:NE	2.35	0.41
1:B:175:PHE:CE1	1:B:216:VAL:HG11	2.52	0.41
1:E:169:GLU:HB3	1:E:196:LEU:HD21	2.02	0.40

All (1) 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)
1:E:210:ASP:OD1	3:A:225:HOH:O[4_646]	2.13	0.07

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	120/118 (102%)	115 (96%)	5 (4%)	0	100	100
1	B	113/118 (96%)	112 (99%)	1 (1%)	0	100	100
1	C	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
1	D	121/118 (102%)	121 (100%)	0	0	100	100
1	E	115/118 (98%)	113 (98%)	1 (1%)	1 (1%)	21	7
1	F	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
All	All	698/708 (99%)	686 (98%)	11 (2%)	1 (0%)	52	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	120	ARG

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	103/96 (107%)	101 (98%)	2 (2%)	65	52
1	B	95/96 (99%)	93 (98%)	2 (2%)	61	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	98/96 (102%)	96 (98%)	2 (2%)	63	49
1	D	104/96 (108%)	97 (93%)	7 (7%)	20	6
1	E	96/96 (100%)	91 (95%)	5 (5%)	29	12
1	F	98/96 (102%)	96 (98%)	2 (2%)	63	49
All	All	594/576 (103%)	574 (97%)	20 (3%)	55	26

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143[A]	VAL
1	A	143[B]	VAL
1	B	202	THR
1	B	214	LEU
1	C	120	ARG
1	C	211	SER
1	D	143[A]	VAL
1	D	143[B]	VAL
1	D	152[A]	ARG
1	D	152[B]	ARG
1	D	161[A]	ARG
1	D	161[B]	ARG
1	D	211	SER
1	E	120	ARG
1	E	143[A]	VAL
1	E	143[B]	VAL
1	E	192[A]	ARG
1	E	192[B]	ARG
1	F	152[A]	ARG
1	F	152[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

6 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	3PB	A	301	-	7,10,10	0.75	0	7,14,14	1.15	0
2	3PB	B	301	-	7,10,10	0.65	0	7,14,14	1.46	2 (28%)
2	3PB	C	301	-	7,10,10	0.70	0	7,14,14	1.47	2 (28%)
2	3PB	D	301	-	7,10,10	0.72	0	7,14,14	1.54	2 (28%)
2	3PB	E	301	-	7,10,10	0.57	0	7,14,14	1.35	1 (14%)
2	3PB	F	301	-	7,10,10	0.72	0	7,14,14	1.30	2 (28%)

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	3PB	A	301	-	-	0/7/9/9	0/0/0/0
2	3PB	B	301	-	-	0/7/9/9	0/0/0/0
2	3PB	C	301	-	-	0/7/9/9	0/0/0/0
2	3PB	D	301	-	-	0/7/9/9	0/0/0/0
2	3PB	E	301	-	-	0/7/9/9	0/0/0/0
2	3PB	F	301	-	-	0/7/9/9	0/0/0/0

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	3PB	C4-C3-C2	-2.94	108.73	112.75
2	E	301	3PB	C4-C3-C2	-2.48	109.35	112.75
2	B	301	3PB	C4-C3-C2	-2.39	109.48	112.75
2	C	301	3PB	C4-C3-C2	-2.32	109.58	112.75
2	F	301	3PB	O1P-P-O2P	-2.11	101.83	107.11
2	C	301	3PB	O1P-P-O2P	-2.10	101.86	107.11
2	F	301	3PB	O4P-P-O2P	2.07	117.23	110.58
2	D	301	3PB	O4P-P-O3P	2.34	116.29	107.38
2	B	301	3PB	O4P-P-O3P	2.98	118.71	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	104/118 (88%)	-0.07	3 (2%) 55 49	8, 12, 21, 48	0
1	B	103/118 (87%)	0.20	6 (5%) 26 21	9, 14, 24, 49	0
1	C	103/118 (87%)	0.07	6 (5%) 26 21	9, 13, 22, 46	0
1	D	104/118 (88%)	0.04	3 (2%) 55 49	9, 15, 23, 49	0
1	E	103/118 (87%)	0.19	5 (4%) 33 27	7, 14, 23, 38	0
1	F	103/118 (87%)	0.06	5 (4%) 33 27	10, 15, 25, 48	0
All	All	620/708 (87%)	0.08	28 (4%) 37 31	7, 14, 24, 49	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	223	ALA	9.1
1	B	223	ALA	8.5
1	F	223	ALA	7.2
1	E	223	ALA	7.1
1	A	223	ALA	6.2
1	C	118	SER	5.5
1	E	221	VAL	5.0
1	B	222	THR	4.7
1	D	224	GLU	4.2
1	B	224	GLU	4.1
1	F	224	GLU	3.9
1	D	119	GLY	3.7
1	C	222	THR	3.7
1	C	119	GLY	3.6
1	C	221	VAL	3.0
1	A	224	GLU	3.0
1	E	222	THR	3.0
1	E	192[A]	ARG	2.9
1	C	120	ARG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	119	GLY	2.6
1	B	221	VAL	2.6
1	F	161[A]	ARG	2.5
1	F	120	ARG	2.5
1	C	200	GLY	2.5
1	B	202	THR	2.4
1	A	119	GLY	2.3
1	F	222	THR	2.2
1	B	212[A]	GLY	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	3PB	F	301	11/11	0.88	0.23	8.40	10,12,23,26	11
2	3PB	B	301	11/11	0.88	0.28	7.91	9,12,22,24	11
2	3PB	D	301	11/11	0.92	0.16	4.18	13,16,29,31	11
2	3PB	E	301	11/11	0.79	0.24	4.09	18,21,31,33	11
2	3PB	A	301	11/11	0.89	0.16	3.61	10,13,23,27	11
2	3PB	C	301	11/11	0.88	0.20	2.19	8,11,25,27	11

6.5 Other polymers [i](#)

There are no such residues in this entry.