wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	3GQQ
Title	:	Crystal structure of the human retinal protein 4 (unc-119 homolog A). Northeast Structural Genomics Consortium target HR3066a
Authors	:	Vorobiev, S.M.; Chen, Y.; Seetharaman, J.; Shastry, R.; Foote, E.L.; Ciccosanti, C.; Sahdev, S.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2009-03-24
Resolution	:	1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

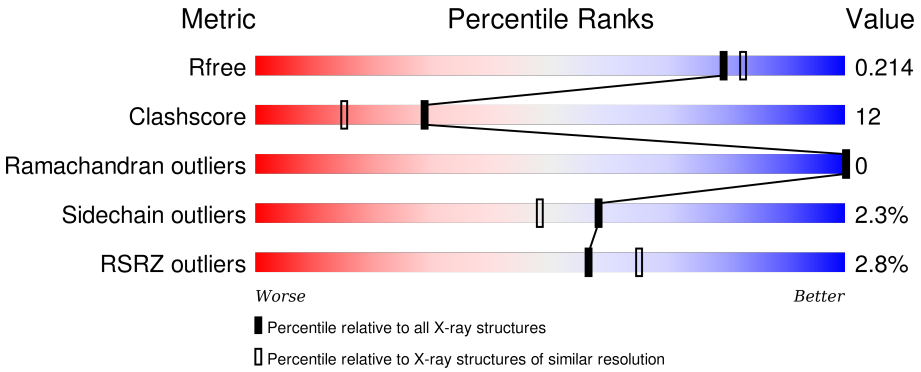
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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 <=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	195	69% 16% • 14%
1	B	195	3% 78% 12% • 9%
1	C	195	3% 68% 18% • 13%
1	D	195	3% 74% 18% • 7%
1	E	195	2% 67% 15% • 15%

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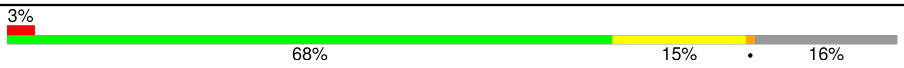
Mol	Chain	Length	Quality of chain
1	F	195	

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	UNL	A	401	-	-	-	X
2	UNL	B	410	-	-	-	X
2	UNL	B	412	-	-	-	X
2	UNL	B	413	-	-	-	X
2	UNL	C	421	-	-	-	X
2	UNL	C	422	-	-	-	X
2	UNL	D	431	-	-	-	X
2	UNL	D	433	-	-	-	X
2	UNL	E	441	-	-	-	X
2	UNL	E	442	-	-	-	X
2	UNL	E	443	-	-	-	X
2	UNL	E	446	-	-	-	X
2	UNL	F	452	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9290 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 Protein unc-119 homolog A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	Se	0	0	0
			1378	887	232	252	3	4			
1	B	178	Total	C	N	O	S	Se	0	0	0
			1458	936	247	268	3	4			
1	C	170	Total	C	N	O	S	Se	0	0	0
			1408	907	238	256	3	4			
1	D	181	Total	C	N	O	S	Se	0	0	0
			1483	953	252	271	3	4			
1	E	165	Total	C	N	O	S	Se	0	0	0
			1367	880	229	251	3	4			
1	F	164	Total	C	N	O	S	Se	0	0	0
			1363	879	229	248	3	4			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	MSE	-	EXPRESSION TAG	UNP Q13432
A	47	GLY	-	EXPRESSION TAG	UNP Q13432
A	48	HIS	-	EXPRESSION TAG	UNP Q13432
A	49	HIS	-	EXPRESSION TAG	UNP Q13432
A	50	HIS	-	EXPRESSION TAG	UNP Q13432
A	51	HIS	-	EXPRESSION TAG	UNP Q13432
A	52	HIS	-	EXPRESSION TAG	UNP Q13432
A	53	HIS	-	EXPRESSION TAG	UNP Q13432
A	54	SER	-	EXPRESSION TAG	UNP Q13432
A	55	HIS	-	EXPRESSION TAG	UNP Q13432
B	46	MSE	-	EXPRESSION TAG	UNP Q13432
B	47	GLY	-	EXPRESSION TAG	UNP Q13432
B	48	HIS	-	EXPRESSION TAG	UNP Q13432
B	49	HIS	-	EXPRESSION TAG	UNP Q13432
B	50	HIS	-	EXPRESSION TAG	UNP Q13432
B	51	HIS	-	EXPRESSION TAG	UNP Q13432
B	52	HIS	-	EXPRESSION TAG	UNP Q13432

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Chain	Residue	Modelled	Actual	Comment	Reference
B	53	HIS	-	EXPRESSION TAG	UNP Q13432
B	54	SER	-	EXPRESSION TAG	UNP Q13432
B	55	HIS	-	EXPRESSION TAG	UNP Q13432
C	46	MSE	-	EXPRESSION TAG	UNP Q13432
C	47	GLY	-	EXPRESSION TAG	UNP Q13432
C	48	HIS	-	EXPRESSION TAG	UNP Q13432
C	49	HIS	-	EXPRESSION TAG	UNP Q13432
C	50	HIS	-	EXPRESSION TAG	UNP Q13432
C	51	HIS	-	EXPRESSION TAG	UNP Q13432
C	52	HIS	-	EXPRESSION TAG	UNP Q13432
C	53	HIS	-	EXPRESSION TAG	UNP Q13432
C	54	SER	-	EXPRESSION TAG	UNP Q13432
C	55	HIS	-	EXPRESSION TAG	UNP Q13432
D	46	MSE	-	EXPRESSION TAG	UNP Q13432
D	47	GLY	-	EXPRESSION TAG	UNP Q13432
D	48	HIS	-	EXPRESSION TAG	UNP Q13432
D	49	HIS	-	EXPRESSION TAG	UNP Q13432
D	50	HIS	-	EXPRESSION TAG	UNP Q13432
D	51	HIS	-	EXPRESSION TAG	UNP Q13432
D	52	HIS	-	EXPRESSION TAG	UNP Q13432
D	53	HIS	-	EXPRESSION TAG	UNP Q13432
D	54	SER	-	EXPRESSION TAG	UNP Q13432
D	55	HIS	-	EXPRESSION TAG	UNP Q13432
E	46	MSE	-	EXPRESSION TAG	UNP Q13432
E	47	GLY	-	EXPRESSION TAG	UNP Q13432
E	48	HIS	-	EXPRESSION TAG	UNP Q13432
E	49	HIS	-	EXPRESSION TAG	UNP Q13432
E	50	HIS	-	EXPRESSION TAG	UNP Q13432
E	51	HIS	-	EXPRESSION TAG	UNP Q13432
E	52	HIS	-	EXPRESSION TAG	UNP Q13432
E	53	HIS	-	EXPRESSION TAG	UNP Q13432
E	54	SER	-	EXPRESSION TAG	UNP Q13432
E	55	HIS	-	EXPRESSION TAG	UNP Q13432
F	46	MSE	-	EXPRESSION TAG	UNP Q13432
F	47	GLY	-	EXPRESSION TAG	UNP Q13432
F	48	HIS	-	EXPRESSION TAG	UNP Q13432
F	49	HIS	-	EXPRESSION TAG	UNP Q13432
F	50	HIS	-	EXPRESSION TAG	UNP Q13432
F	51	HIS	-	EXPRESSION TAG	UNP Q13432
F	52	HIS	-	EXPRESSION TAG	UNP Q13432
F	53	HIS	-	EXPRESSION TAG	UNP Q13432
F	54	SER	-	EXPRESSION TAG	UNP Q13432

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Chain	Residue	Modelled	Actual	Comment	Reference
F	55	HIS	-	EXPRESSION TAG	UNP Q13432

- Molecule 2 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

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

- Molecule 3 is water.

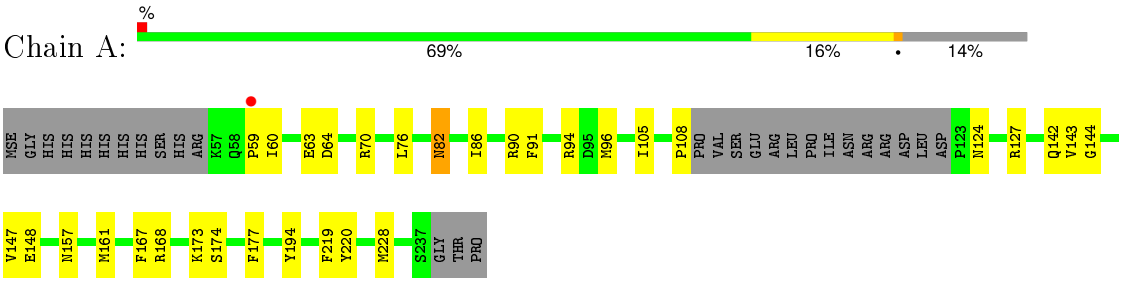
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	160	Total O 160 160	0	0
3	B	134	Total O 134 134	0	0
3	C	155	Total O 155 155	0	0
3	D	158	Total O 158 158	0	0
3	E	108	Total O 108 108	0	0
3	F	88	Total O 88 88	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

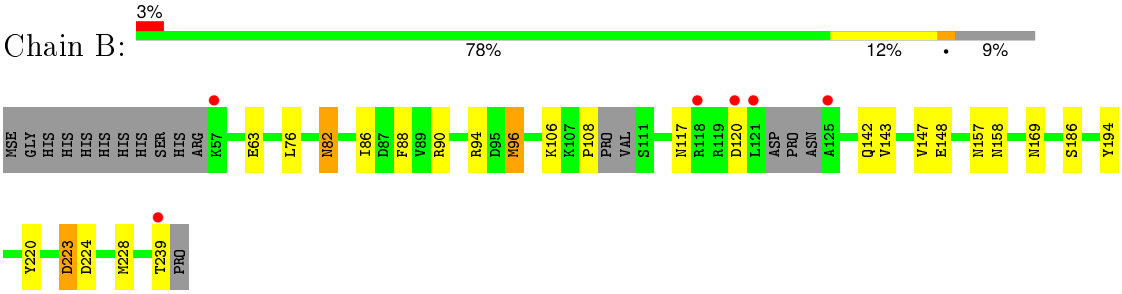
- Molecule 1: Protein unc-119 homolog A

Chain A:



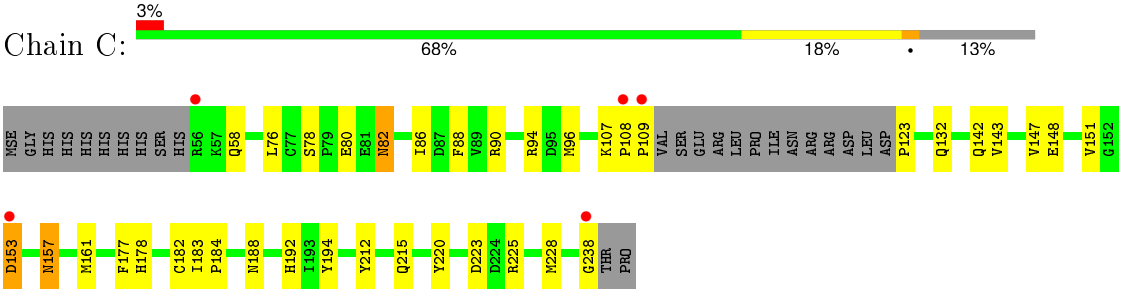
- Molecule 1: Protein unc-119 homolog A

Chain B:



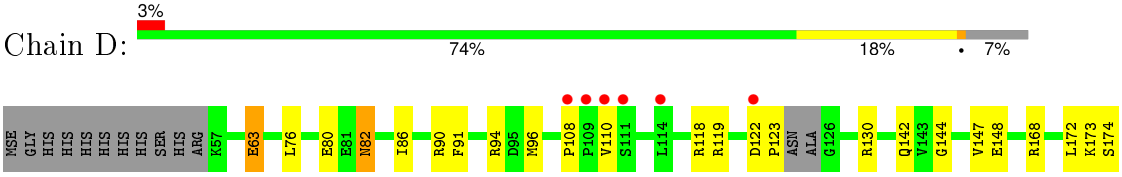
- Molecule 1: Protein unc-119 homolog A

Chain C:



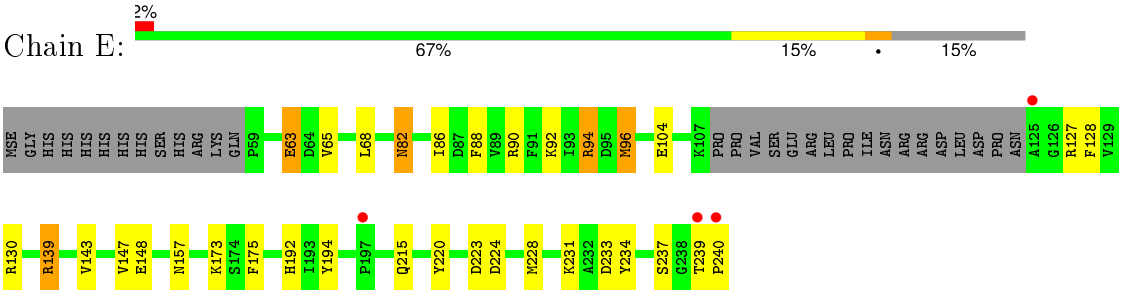
- Molecule 1: Protein unc-119 homolog A

Chain D:



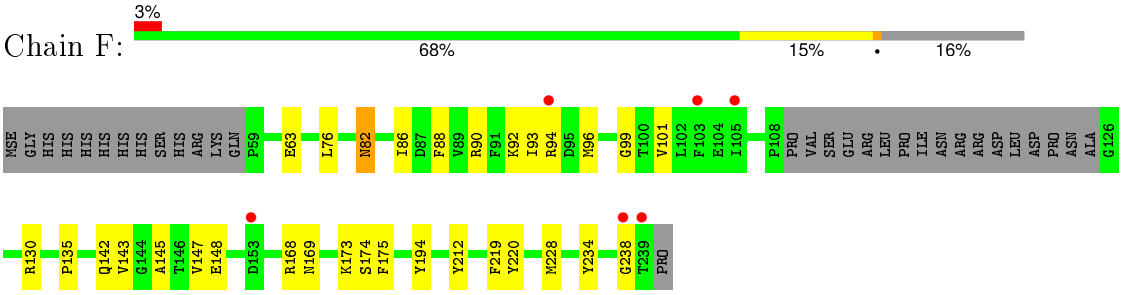
• Molecule 1: Protein unc-119 homolog A

Chain E:



• Molecule 1: Protein unc-119 homolog A

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.89Å 79.56Å 189.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.51 – 1.95 94.86 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.51-1.95) 99.3 (94.86-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 1.94Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.191 , 0.214 0.192 , 0.214	Depositor DCC
R_{free} test set	4351 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.6	EDS
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 86760 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9290	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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 20.35 % 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 8.8646e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: UNL

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	0.34	0/1412	0.62	1/1900 (0.1%)
1	B	0.32	0/1492	0.59	0/2007
1	C	0.33	0/1444	0.58	0/1942
1	D	0.33	0/1520	0.61	0/2050
1	E	0.32	0/1401	0.58	0/1883
1	F	0.31	0/1397	0.57	0/1877
All	All	0.33	0/8666	0.59	1/11659 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	PRO	N-CA-CB	5.60	110.02	103.30

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	1378	0	1310	29	0
1	B	1458	0	1386	25	0
1	C	1408	0	1356	48	0
1	D	1483	0	1414	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1367	0	1309	36	0
1	F	1363	0	1310	25	0
2	A	6	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	6	0	0	1	0
2	E	6	0	0	0	0
2	F	4	0	0	0	0
3	A	160	0	0	3	0
3	B	134	0	0	5	0
3	C	155	0	0	4	0
3	D	158	0	0	1	0
3	E	108	0	0	4	0
3	F	88	0	0	2	0
All	All	9290	0	8085	191	0

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 12.

The worst 5 of 191 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:E:96:MSE:HE2	1:E:96:MSE:HA	1.28	1.08
1:B:96:MSE:HA	1:B:96:MSE:HE2	1.35	1.07
1:E:239:THR:N	1:E:240:PRO:HA	1.75	1.01
1:E:139:ARG:HH11	1:E:139:ARG:HG3	1.26	1.00
1:C:183:ILE:H	1:C:188:ASN:HD21	1.03	0.99

There are no symmetry-related clashes.

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	163/195 (84%)	163 (100%)	0	0	100	100
1	B	172/195 (88%)	166 (96%)	6 (4%)	0	100	100
1	C	166/195 (85%)	165 (99%)	1 (1%)	0	100	100
1	D	177/195 (91%)	174 (98%)	3 (2%)	0	100	100
1	E	161/195 (83%)	158 (98%)	3 (2%)	0	100	100
1	F	160/195 (82%)	159 (99%)	1 (1%)	0	100	100
All	All	999/1170 (85%)	985 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	151/176 (86%)	150 (99%)	1 (1%)	88	87
1	B	159/176 (90%)	155 (98%)	4 (2%)	55	44
1	C	156/176 (89%)	151 (97%)	5 (3%)	46	32
1	D	163/176 (93%)	160 (98%)	3 (2%)	66	58
1	E	151/176 (86%)	145 (96%)	6 (4%)	38	22
1	F	151/176 (86%)	149 (99%)	2 (1%)	76	71
All	All	931/1056 (88%)	910 (98%)	21 (2%)	58	48

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	157	ASN
1	D	76	LEU
1	E	139	ARG
1	C	153	ASP
1	E	237	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	188	ASN
1	D	142	GLN
1	F	142	GLN
1	C	192	HIS
1	D	157	ASN

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

Of 30 ligands modelled in this entry, 30 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	163/195 (83%)	-0.03	1 (0%)	90	93	14, 24, 42, 69	0
1	B	174/195 (89%)	0.19	6 (3%)	49	58	16, 31, 74, 90	0
1	C	166/195 (85%)	0.13	5 (3%)	54	62	15, 29, 55, 102	0
1	D	177/195 (90%)	0.09	6 (3%)	49	58	13, 26, 56, 83	0
1	E	161/195 (82%)	0.14	4 (2%)	61	69	16, 33, 61, 107	0
1	F	160/195 (82%)	0.29	6 (3%)	44	54	18, 41, 68, 102	0
All	All	1001/1170 (85%)	0.14	28 (2%)	56	65	13, 30, 64, 107	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	121	LEU	10.2
1	C	56	ARG	6.1
1	E	239	THR	5.7
1	C	238	GLY	5.0
1	E	125	ALA	5.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	UNL	B	410	1/-	0.80	0.47	42.33	59,59,59,59	0
2	UNL	E	442	1/-	0.81	0.47	31.04	57,57,57,57	0
2	UNL	C	421	1/-	0.80	0.48	29.46	55,55,55,55	0
2	UNL	A	401	1/-	0.80	0.63	25.10	60,60,60,60	0
2	UNL	C	422	1/-	0.81	0.47	19.60	54,54,54,54	0
2	UNL	B	412	1/-	0.89	0.33	14.33	46,46,46,46	0
2	UNL	E	443	1/-	0.95	0.26	10.73	46,46,46,46	0
2	UNL	D	431	1/-	0.88	0.33	9.65	54,54,54,54	0
2	UNL	F	452	1/-	0.73	0.41	9.25	66,66,66,66	0
2	UNL	E	441	1/-	0.60	0.39	9.18	53,53,53,53	0
2	UNL	E	446	1/-	0.99	0.22	7.79	25,25,25,25	0
2	UNL	B	413	1/-	0.78	0.21	5.77	47,47,47,47	0
2	UNL	D	433	1/-	0.94	0.18	3.10	52,52,52,52	0
2	UNL	E	445	1/-	0.98	0.20	2.00	31,31,31,31	0
2	UNL	A	402	1/-	0.94	0.23	-	36,36,36,36	0
2	UNL	D	434	1/-	0.95	0.17	-	40,40,40,40	0
2	UNL	E	444	1/-	0.83	0.17	-	50,50,50,50	0
2	UNL	F	453	1/-	0.60	0.41	-	58,58,58,58	0
2	UNL	C	423	1/-	0.46	0.41	-	49,49,49,49	0
2	UNL	A	404	1/-	0.81	0.23	-	38,38,38,38	0
2	UNL	C	424	1/-	0.95	0.14	-	31,31,31,31	0
2	UNL	F	454	1/-	0.95	0.14	-	37,37,37,37	0
2	UNL	A	405	1/-	0.67	0.32	-	53,53,53,53	0
2	UNL	B	411	1/-	0.82	0.51	-	66,66,66,66	0
2	UNL	D	436	1/-	0.71	0.34	-	52,52,52,52	0
2	UNL	D	435	1/-	0.77	0.29	-	38,38,38,38	0
2	UNL	F	451	1/-	0.90	0.48	-	62,62,62,62	0
2	UNL	D	432	1/-	0.90	0.23	-	52,52,52,52	0
2	UNL	A	403	1/-	0.86	0.32	-	48,48,48,48	0
2	UNL	A	406	1/-	0.94	0.22	-	32,32,32,32	0

6.5 Other polymers

There are no such residues in this entry.