wwPDB X-ray Structure Validation Summary Report (i)

Mar 13, 2023 – 12:41 pm GMT

PDB ID	:	7Z3Q
Title	:	Crystal structure of the human leptin:LepR-CRH2 encounter complex to 3.6 A resolution.
Authors	:	Verstraete, K.; Verschueren, K.; Alexandra, T.; Savvides, S.N.
Deposited on	:	2022-03-02
Resolution	:	3.62 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

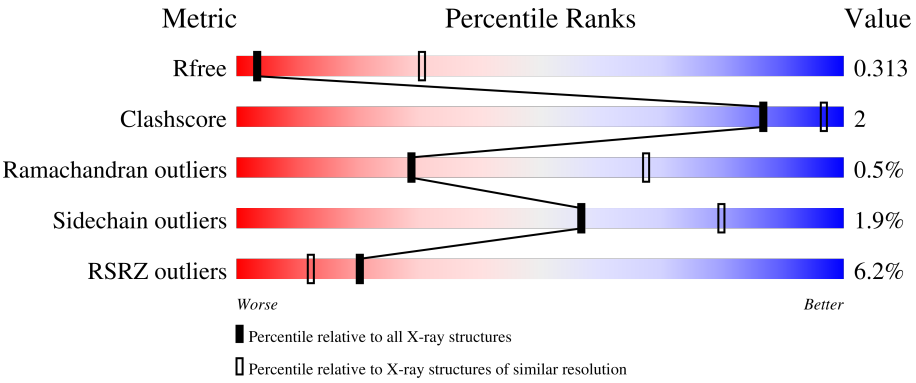
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 3.62 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}	130704	1290 (3.74-3.50)
Clashscore	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)
RSRZ outliers	127900	1191 (3.74-3.50)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	171	49% 6% 45%
1	C	171	51% 7% 42%
1	E	171	52% 8% 40%
2	B	232	82% 13%
2	D	232	8% 80% 5% 14%

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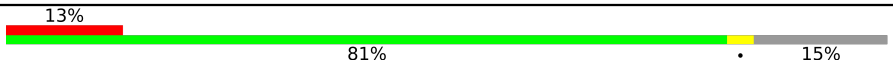
Mol	Chain	Length	Quality of chain
2	F	232	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7102 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 Leptin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	S	0	0	0
			744	468	127	146	3			
1	C	100	Total	C	N	O	S	0	0	0
			787	494	135	153	5			
1	E	102	Total	C	N	O	S	0	0	0
			801	504	137	155	5			

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP P41159
A	-2	HIS	-	expression tag	UNP P41159
A	-1	HIS	-	expression tag	UNP P41159
A	0	HIS	-	expression tag	UNP P41159
A	1	HIS	-	expression tag	UNP P41159
A	2	HIS	-	expression tag	UNP P41159
A	3	HIS	-	expression tag	UNP P41159
A	4	PRO	-	expression tag	UNP P41159
A	5	GLY	-	expression tag	UNP P41159
A	6	GLY	-	expression tag	UNP P41159
A	7	PRO	-	expression tag	UNP P41159
A	8	GLY	-	expression tag	UNP P41159
A	9	SER	-	expression tag	UNP P41159
A	10	GLU	-	expression tag	UNP P41159
A	11	ASN	-	expression tag	UNP P41159
A	12	LEU	-	expression tag	UNP P41159
A	13	TYR	-	expression tag	UNP P41159
A	14	PHE	-	expression tag	UNP P41159
A	15	GLN	-	expression tag	UNP P41159
A	16	GLY	-	expression tag	UNP P41159
A	17	GLY	-	expression tag	UNP P41159
A	18	SER	-	expression tag	UNP P41159
A	19	THR	-	expression tag	UNP P41159

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Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLY	-	expression tag	UNP P41159
A	21	GLY	-	expression tag	UNP P41159
C	-3	ALA	-	expression tag	UNP P41159
C	-2	HIS	-	expression tag	UNP P41159
C	-1	HIS	-	expression tag	UNP P41159
C	0	HIS	-	expression tag	UNP P41159
C	1	HIS	-	expression tag	UNP P41159
C	2	HIS	-	expression tag	UNP P41159
C	3	HIS	-	expression tag	UNP P41159
C	4	PRO	-	expression tag	UNP P41159
C	5	GLY	-	expression tag	UNP P41159
C	6	GLY	-	expression tag	UNP P41159
C	7	PRO	-	expression tag	UNP P41159
C	8	GLY	-	expression tag	UNP P41159
C	9	SER	-	expression tag	UNP P41159
C	10	GLU	-	expression tag	UNP P41159
C	11	ASN	-	expression tag	UNP P41159
C	12	LEU	-	expression tag	UNP P41159
C	13	TYR	-	expression tag	UNP P41159
C	14	PHE	-	expression tag	UNP P41159
C	15	GLN	-	expression tag	UNP P41159
C	16	GLY	-	expression tag	UNP P41159
C	17	GLY	-	expression tag	UNP P41159
C	18	SER	-	expression tag	UNP P41159
C	19	THR	-	expression tag	UNP P41159
C	20	GLY	-	expression tag	UNP P41159
C	21	GLY	-	expression tag	UNP P41159
E	-3	ALA	-	expression tag	UNP P41159
E	-2	HIS	-	expression tag	UNP P41159
E	-1	HIS	-	expression tag	UNP P41159
E	0	HIS	-	expression tag	UNP P41159
E	1	HIS	-	expression tag	UNP P41159
E	2	HIS	-	expression tag	UNP P41159
E	3	HIS	-	expression tag	UNP P41159
E	4	PRO	-	expression tag	UNP P41159
E	5	GLY	-	expression tag	UNP P41159
E	6	GLY	-	expression tag	UNP P41159
E	7	PRO	-	expression tag	UNP P41159
E	8	GLY	-	expression tag	UNP P41159
E	9	SER	-	expression tag	UNP P41159
E	10	GLU	-	expression tag	UNP P41159
E	11	ASN	-	expression tag	UNP P41159

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Chain	Residue	Modelled	Actual	Comment	Reference
E	12	LEU	-	expression tag	UNP P41159
E	13	TYR	-	expression tag	UNP P41159
E	14	PHE	-	expression tag	UNP P41159
E	15	GLN	-	expression tag	UNP P41159
E	16	GLY	-	expression tag	UNP P41159
E	17	GLY	-	expression tag	UNP P41159
E	18	SER	-	expression tag	UNP P41159
E	19	THR	-	expression tag	UNP P41159
E	20	GLY	-	expression tag	UNP P41159
E	21	GLY	-	expression tag	UNP P41159

- Molecule 2 is a protein called Leptin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	201	Total	C	N	O	S	0	0	0
			1605	1034	260	301	10			
2	D	199	Total	C	N	O	S	0	0	0
			1588	1023	258	297	10			
2	F	197	Total	C	N	O	S	0	0	0
			1575	1016	256	293	10			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	404	ALA	-	expression tag	UNP P48357
B	405	HIS	-	expression tag	UNP P48357
B	406	HIS	-	expression tag	UNP P48357
B	407	HIS	-	expression tag	UNP P48357
B	408	HIS	-	expression tag	UNP P48357
B	409	HIS	-	expression tag	UNP P48357
B	410	HIS	-	expression tag	UNP P48357
B	411	PRO	-	expression tag	UNP P48357
B	412	GLY	-	expression tag	UNP P48357
B	413	GLY	-	expression tag	UNP P48357
B	414	PRO	-	expression tag	UNP P48357
B	415	GLY	-	expression tag	UNP P48357
B	416	SER	-	expression tag	UNP P48357
B	417	GLU	-	expression tag	UNP P48357
B	418	ASN	-	expression tag	UNP P48357
B	419	LEU	-	expression tag	UNP P48357
B	420	TYR	-	expression tag	UNP P48357
B	421	PHE	-	expression tag	UNP P48357

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Chain	Residue	Modelled	Actual	Comment	Reference
B	422	GLN	-	expression tag	UNP P48357
B	423	GLY	-	expression tag	UNP P48357
B	424	GLY	-	expression tag	UNP P48357
B	425	SER	-	expression tag	UNP P48357
B	426	SER	-	expression tag	UNP P48357
B	427	GLY	-	expression tag	UNP P48357
B	516	GLN	ASN	conflict	UNP P48357
B	604	SER	CYS	conflict	UNP P48357
D	404	ALA	-	expression tag	UNP P48357
D	405	HIS	-	expression tag	UNP P48357
D	406	HIS	-	expression tag	UNP P48357
D	407	HIS	-	expression tag	UNP P48357
D	408	HIS	-	expression tag	UNP P48357
D	409	HIS	-	expression tag	UNP P48357
D	410	HIS	-	expression tag	UNP P48357
D	411	PRO	-	expression tag	UNP P48357
D	412	GLY	-	expression tag	UNP P48357
D	413	GLY	-	expression tag	UNP P48357
D	414	PRO	-	expression tag	UNP P48357
D	415	GLY	-	expression tag	UNP P48357
D	416	SER	-	expression tag	UNP P48357
D	417	GLU	-	expression tag	UNP P48357
D	418	ASN	-	expression tag	UNP P48357
D	419	LEU	-	expression tag	UNP P48357
D	420	TYR	-	expression tag	UNP P48357
D	421	PHE	-	expression tag	UNP P48357
D	422	GLN	-	expression tag	UNP P48357
D	423	GLY	-	expression tag	UNP P48357
D	424	GLY	-	expression tag	UNP P48357
D	425	SER	-	expression tag	UNP P48357
D	426	SER	-	expression tag	UNP P48357
D	427	GLY	-	expression tag	UNP P48357
D	516	GLN	ASN	conflict	UNP P48357
D	604	SER	CYS	conflict	UNP P48357
F	404	ALA	-	expression tag	UNP P48357
F	405	HIS	-	expression tag	UNP P48357
F	406	HIS	-	expression tag	UNP P48357
F	407	HIS	-	expression tag	UNP P48357
F	408	HIS	-	expression tag	UNP P48357
F	409	HIS	-	expression tag	UNP P48357
F	410	HIS	-	expression tag	UNP P48357
F	411	PRO	-	expression tag	UNP P48357

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Chain	Residue	Modelled	Actual	Comment	Reference
F	412	GLY	-	expression tag	UNP P48357
F	413	GLY	-	expression tag	UNP P48357
F	414	PRO	-	expression tag	UNP P48357
F	415	GLY	-	expression tag	UNP P48357
F	416	SER	-	expression tag	UNP P48357
F	417	GLU	-	expression tag	UNP P48357
F	418	ASN	-	expression tag	UNP P48357
F	419	LEU	-	expression tag	UNP P48357
F	420	TYR	-	expression tag	UNP P48357
F	421	PHE	-	expression tag	UNP P48357
F	422	GLN	-	expression tag	UNP P48357
F	423	GLY	-	expression tag	UNP P48357
F	424	GLY	-	expression tag	UNP P48357
F	425	SER	-	expression tag	UNP P48357
F	426	SER	-	expression tag	UNP P48357
F	427	GLY	-	expression tag	UNP P48357
F	516	GLN	ASN	conflict	UNP P48357
F	604	SER	CYS	conflict	UNP P48357

- Molecule 3 is water.

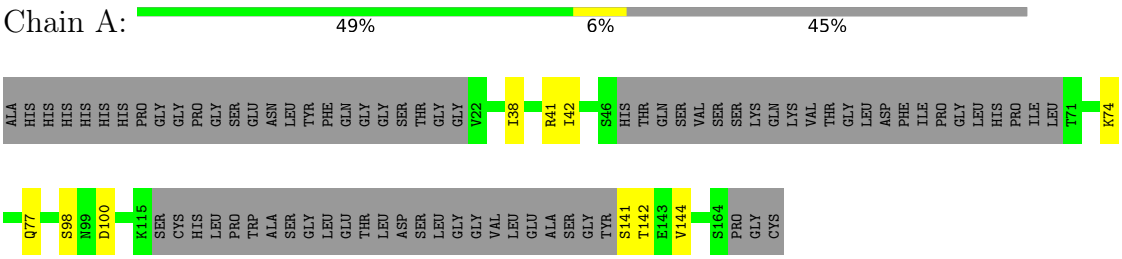
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

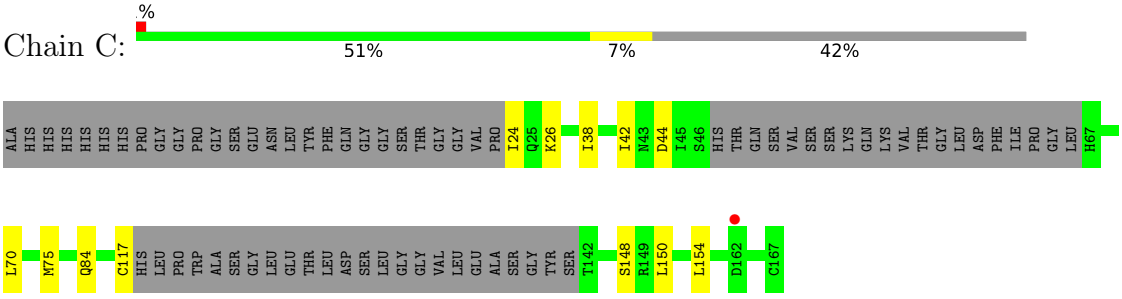
• Molecule 1: Leptin

Chain A:



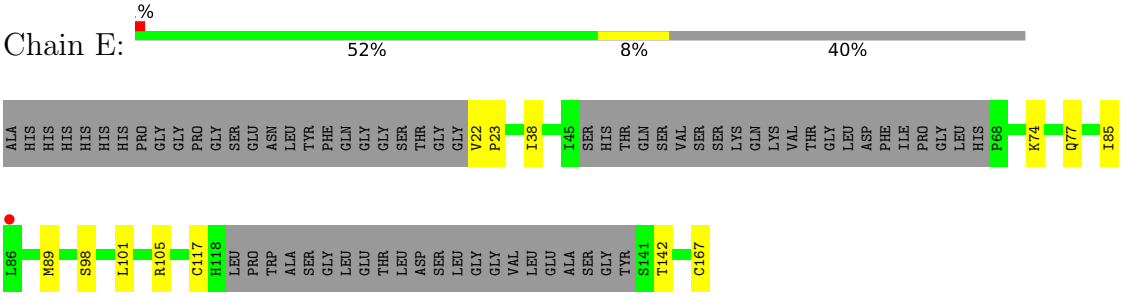
• Molecule 1: Leptin

Chain C:



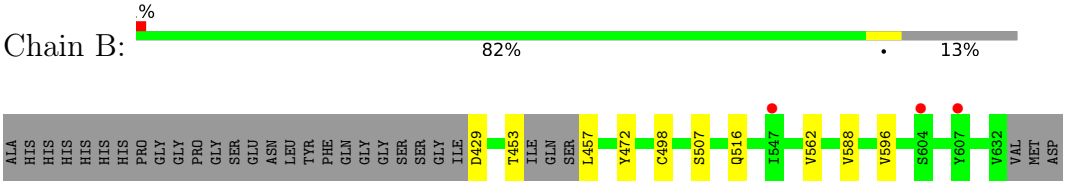
• Molecule 1: Leptin

Chain E:



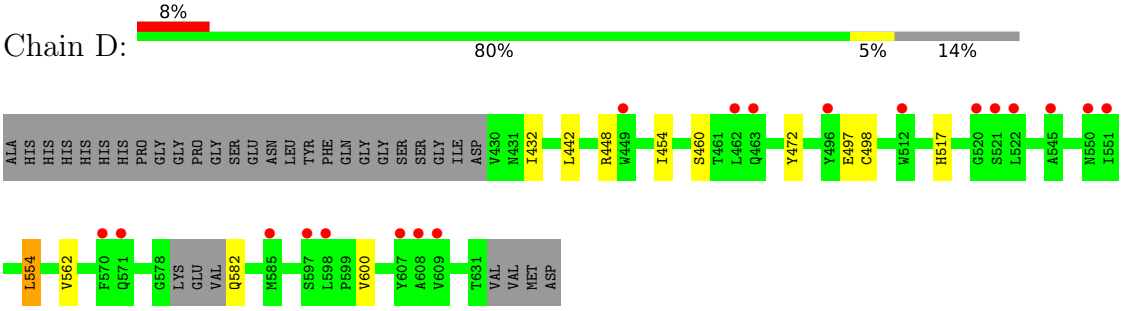
• Molecule 2: Leptin receptor

Chain B:



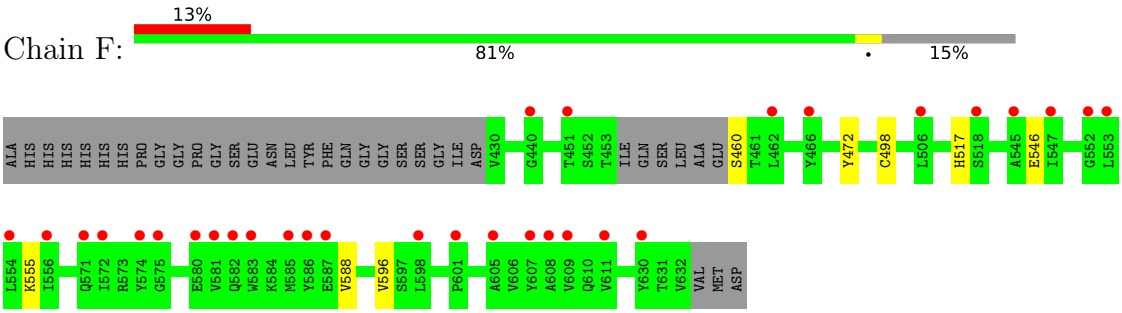
• Molecule 2: Leptin receptor

Chain D:



• Molecule 2: Leptin receptor

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	156.20Å 156.64Å 95.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.57 – 3.62 60.57 – 3.62	Depositor EDS
% Data completeness (in resolution range)	98.9 (60.57-3.62) 98.8 (60.57-3.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.66 (at 3.57Å)	Xtriage
Refinement program	BUSTER 2.10.4 (3-FEB-2022)	Depositor
R, R_{free}	0.275 , 0.305 0.271 , 0.313	Depositor DCC
R_{free} test set	1050 reflections (7.71%)	wwPDB-VP
Wilson B-factor (Å^2)	132.6	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 174.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.034 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7102	wwPDB-VP
Average B, all atoms (Å^2)	185.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

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	0.26	0/748	0.41	0/1011
1	C	0.28	0/793	0.45	0/1071
1	E	0.26	0/808	0.42	0/1092
2	B	0.28	0/1650	0.48	0/2250
2	D	0.25	0/1633	0.45	0/2227
2	F	0.22	0/1620	0.42	0/2209
All	All	0.26	0/7252	0.44	0/9860

There are no bond length outliers.

There are no bond angle outliers.

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	744	0	779	10	0
1	C	787	0	817	6	0
1	E	801	0	834	10	0
2	B	1605	0	1579	2	0
2	D	1588	0	1562	6	0
2	F	1575	0	1553	3	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
All	All	7102	0	7124	30	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 2.

The worst 5 of 30 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:41:ARG:NH2	1:A:100:ASP:OD2	2.30	0.64
2:B:453:THR:HG22	2:B:457:LEU:HD21	1.78	0.64
1:A:38:ILE:O	1:A:42:ILE:HG13	1.99	0.61
2:F:588:VAL:HG21	2:F:596:VAL:HG21	1.81	0.61
1:C:38:ILE:O	1:C:42:ILE:HG12	2.00	0.60

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	88/171 (52%)	88 (100%)	0	0	100	100
1	C	94/171 (55%)	90 (96%)	3 (3%)	1 (1%)	14	53
1	E	96/171 (56%)	94 (98%)	2 (2%)	0	100	100
2	B	197/232 (85%)	193 (98%)	3 (2%)	1 (0%)	29	67
2	D	195/232 (84%)	185 (95%)	9 (5%)	1 (0%)	29	67
2	F	193/232 (83%)	188 (97%)	4 (2%)	1 (0%)	29	67
All	All	863/1209 (71%)	838 (97%)	21 (2%)	4 (0%)	29	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	472	TYR
2	D	472	TYR
2	F	472	TYR

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Mol	Chain	Res	Type
1	C	44	ASP

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	90/150 (60%)	89 (99%)	1 (1%)	73 87
1	C	95/150 (63%)	91 (96%)	4 (4%)	30 63
1	E	97/150 (65%)	96 (99%)	1 (1%)	76 88
2	B	186/210 (89%)	181 (97%)	5 (3%)	44 73
2	D	184/210 (88%)	180 (98%)	4 (2%)	52 77
2	F	183/210 (87%)	182 (100%)	1 (0%)	88 95
All	All	835/1080 (77%)	819 (98%)	16 (2%)	57 80

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	98	SER
2	D	582	GLN
1	C	117	CYS
2	D	562	VAL
1	C	26	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	517	HIS
1	E	77	GLN
2	D	480	HIS
1	C	84	GLN
2	D	517	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	94/171 (54%)	-0.09	0 100 100	109, 155, 221, 252	0
1	C	100/171 (58%)	0.08	1 (1%) 82 70	98, 154, 222, 261	0
1	E	102/171 (59%)	0.15	1 (0%) 82 70	118, 175, 234, 268	0
2	B	201/232 (86%)	0.11	3 (1%) 73 60	104, 155, 252, 288	0
2	D	199/232 (85%)	0.54	19 (9%) 8 4	114, 191, 291, 300	0
2	F	197/232 (84%)	0.70	31 (15%) 2 1	110, 220, 298, 300	0
All	All	893/1209 (73%)	0.32	55 (6%) 20 12	98, 175, 285, 300	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	545	ALA	6.4
2	D	521	SER	6.4
2	F	545	ALA	4.9
2	D	520	GLY	4.7
2	F	554	LEU	4.3

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.