Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2024 – 04:07 PM JST

PDB ID	:	8IVD
Title	:	COMPLEX STRUCTURE OF CD93-IGFBP7
Authors	:	Xu, Y.M.; Song, G.J.
Deposited on	:	2023-03-27
Resolution	:	3.24 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

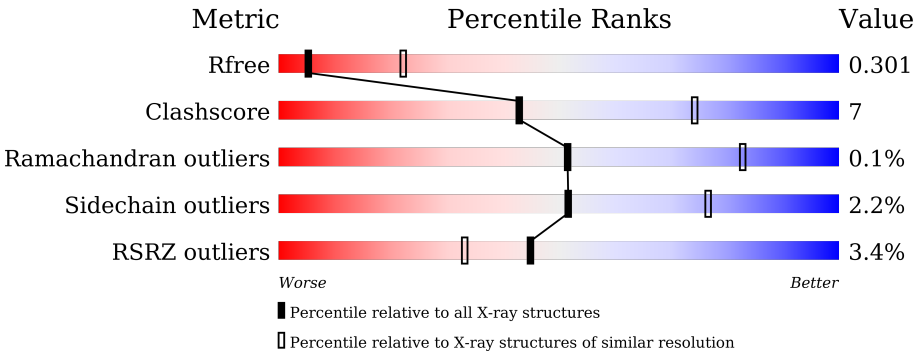
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

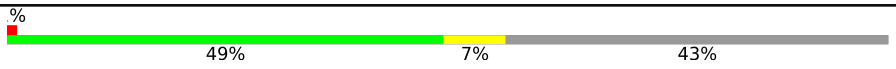
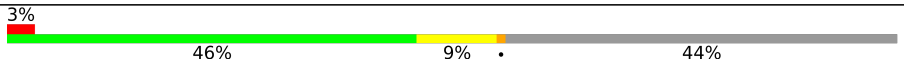
The reported resolution of this entry is 3.24 Å.

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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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	481	
1	B	481	
1	C	481	
1	D	481	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5380 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 Insulin-like growth factor-binding protein 7,Complement component C1q receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			1961	1224	337	380	20			
1	B	267	Total	C	N	O	S	0	0	0
			1917	1193	337	368	19			
1	C	115	Total	C	N	O	S	0	0	0
			766	455	139	154	18			
1	D	108	Total	C	N	O	S	0	0	0
			719	429	126	146	18			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-125	ASP	-	expression tag	UNP Q16270
A	-124	TYR	-	expression tag	UNP Q16270
A	-123	LYS	-	expression tag	UNP Q16270
A	-122	ASP	-	expression tag	UNP Q16270
A	-121	ASP	-	expression tag	UNP Q16270
A	-120	ASP	-	expression tag	UNP Q16270
A	-119	ASP	-	expression tag	UNP Q16270
A	-118	ALA	-	expression tag	UNP Q16270
A	13	GLY	-	linker	UNP Q16270
A	14	SER	-	linker	UNP Q16270
A	15	GLY	-	linker	UNP Q16270
A	16	GLY	-	linker	UNP Q16270
A	17	SER	-	linker	UNP Q16270
A	18	SER	-	linker	UNP Q16270
A	19	GLY	-	linker	UNP Q16270
A	20	GLY	-	linker	UNP Q16270
A	21	SER	-	linker	UNP Q16270
A	22	GLY	-	linker	UNP Q16270
A	23	SER	-	linker	UNP Q16270
A	24	GLY	-	linker	UNP Q16270

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Chain	Residue	Modelled	Actual	Comment	Reference
A	348	HIS	-	expression tag	UNP Q9NPY3
A	349	HIS	-	expression tag	UNP Q9NPY3
A	350	HIS	-	expression tag	UNP Q9NPY3
A	351	HIS	-	expression tag	UNP Q9NPY3
A	352	HIS	-	expression tag	UNP Q9NPY3
A	353	HIS	-	expression tag	UNP Q9NPY3
A	354	HIS	-	expression tag	UNP Q9NPY3
A	355	ALA	-	expression tag	UNP Q9NPY3
B	-125	ASP	-	expression tag	UNP Q16270
B	-124	TYR	-	expression tag	UNP Q16270
B	-123	LYS	-	expression tag	UNP Q16270
B	-122	ASP	-	expression tag	UNP Q16270
B	-121	ASP	-	expression tag	UNP Q16270
B	-120	ASP	-	expression tag	UNP Q16270
B	-119	ASP	-	expression tag	UNP Q16270
B	-118	ALA	-	expression tag	UNP Q16270
B	13	GLY	-	linker	UNP Q16270
B	14	SER	-	linker	UNP Q16270
B	15	GLY	-	linker	UNP Q16270
B	16	GLY	-	linker	UNP Q16270
B	17	SER	-	linker	UNP Q16270
B	18	SER	-	linker	UNP Q16270
B	19	GLY	-	linker	UNP Q16270
B	20	GLY	-	linker	UNP Q16270
B	21	SER	-	linker	UNP Q16270
B	22	GLY	-	linker	UNP Q16270
B	23	SER	-	linker	UNP Q16270
B	24	GLY	-	linker	UNP Q16270
B	348	HIS	-	expression tag	UNP Q9NPY3
B	349	HIS	-	expression tag	UNP Q9NPY3
B	350	HIS	-	expression tag	UNP Q9NPY3
B	351	HIS	-	expression tag	UNP Q9NPY3
B	352	HIS	-	expression tag	UNP Q9NPY3
B	353	HIS	-	expression tag	UNP Q9NPY3
B	354	HIS	-	expression tag	UNP Q9NPY3
B	355	ALA	-	expression tag	UNP Q9NPY3
C	22	ASP	-	expression tag	UNP Q16270
C	23	TYR	-	expression tag	UNP Q16270
C	24	LYS	-	expression tag	UNP Q16270
C	25	ASP	-	expression tag	UNP Q16270
C	26	ASP	-	expression tag	UNP Q16270
C	27	ASP	-	expression tag	UNP Q16270

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Chain	Residue	Modelled	Actual	Comment	Reference
C	28	ASP	-	expression tag	UNP Q16270
C	29	ALA	-	expression tag	UNP Q16270
C	160	GLY	-	linker	UNP Q16270
C	161	SER	-	linker	UNP Q16270
C	162	GLY	-	linker	UNP Q16270
C	163	GLY	-	linker	UNP Q16270
C	164	SER	-	linker	UNP Q16270
C	165	SER	-	linker	UNP Q16270
C	166	GLY	-	linker	UNP Q16270
C	167	GLY	-	linker	UNP Q16270
C	168	SER	-	linker	UNP Q16270
C	169	GLY	-	linker	UNP Q16270
C	170	SER	-	linker	UNP Q16270
C	171	GLY	-	linker	UNP Q16270
C	495	HIS	-	expression tag	UNP Q9NPY3
C	496	HIS	-	expression tag	UNP Q9NPY3
C	497	HIS	-	expression tag	UNP Q9NPY3
C	498	HIS	-	expression tag	UNP Q9NPY3
C	499	HIS	-	expression tag	UNP Q9NPY3
C	500	HIS	-	expression tag	UNP Q9NPY3
C	501	HIS	-	expression tag	UNP Q9NPY3
C	502	ALA	-	expression tag	UNP Q9NPY3
D	22	ASP	-	expression tag	UNP Q16270
D	23	TYR	-	expression tag	UNP Q16270
D	24	LYS	-	expression tag	UNP Q16270
D	25	ASP	-	expression tag	UNP Q16270
D	26	ASP	-	expression tag	UNP Q16270
D	27	ASP	-	expression tag	UNP Q16270
D	28	ASP	-	expression tag	UNP Q16270
D	29	ALA	-	expression tag	UNP Q16270
D	160	GLY	-	linker	UNP Q16270
D	161	SER	-	linker	UNP Q16270
D	162	GLY	-	linker	UNP Q16270
D	163	GLY	-	linker	UNP Q16270
D	164	SER	-	linker	UNP Q16270
D	165	SER	-	linker	UNP Q16270
D	166	GLY	-	linker	UNP Q16270
D	167	GLY	-	linker	UNP Q16270
D	168	SER	-	linker	UNP Q16270
D	169	GLY	-	linker	UNP Q16270
D	170	SER	-	linker	UNP Q16270
D	171	GLY	-	linker	UNP Q16270

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Chain	Residue	Modelled	Actual	Comment	Reference
D	495	HIS	-	expression tag	UNP Q9NPY3
D	496	HIS	-	expression tag	UNP Q9NPY3
D	497	HIS	-	expression tag	UNP Q9NPY3
D	498	HIS	-	expression tag	UNP Q9NPY3
D	499	HIS	-	expression tag	UNP Q9NPY3
D	500	HIS	-	expression tag	UNP Q9NPY3
D	501	HIS	-	expression tag	UNP Q9NPY3
D	502	ALA	-	expression tag	UNP Q9NPY3

- Molecule 2 is water.

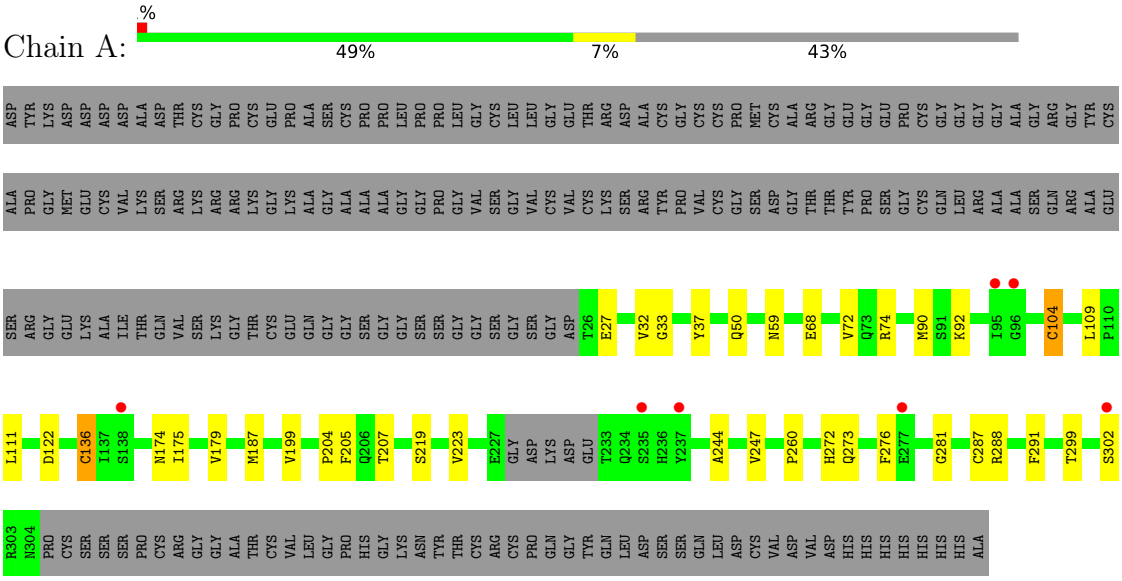
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total O 7 7	0	0
2	B	5	Total O 5 5	0	0
2	C	3	Total O 3 3	0	0
2	D	2	Total O 2 2	0	0

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.

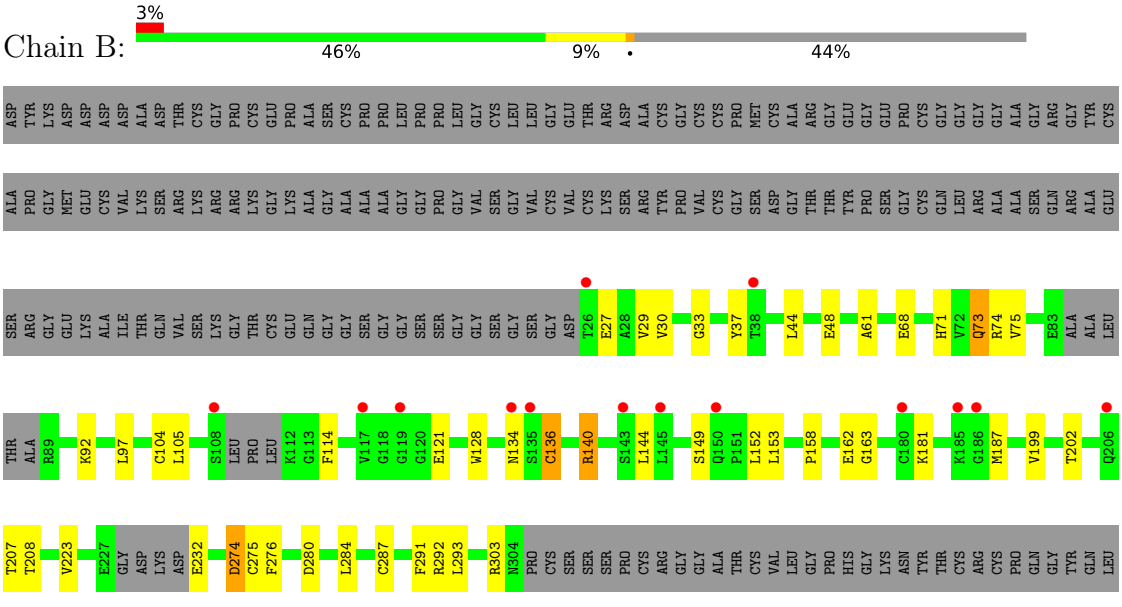
• Molecule 1: Insulin-like growth factor-binding protein 7,Complement component C1q receptor

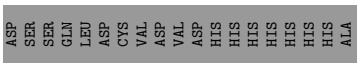
Chain A:



• Molecule 1: Insulin-like growth factor-binding protein 7,Complement component C1q receptor

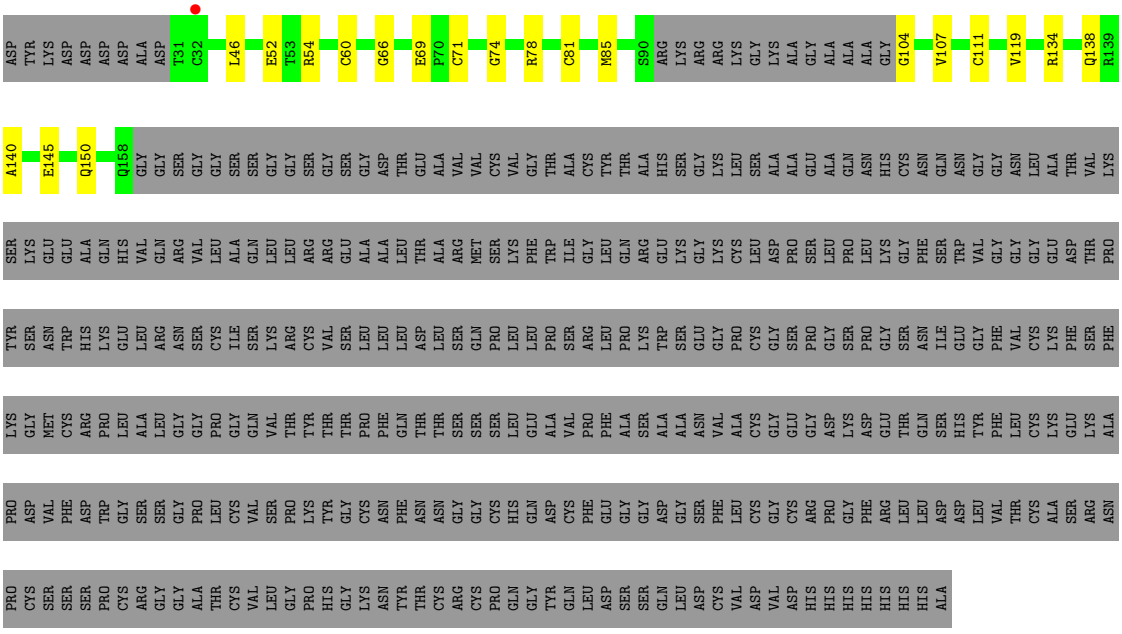
Chain B:





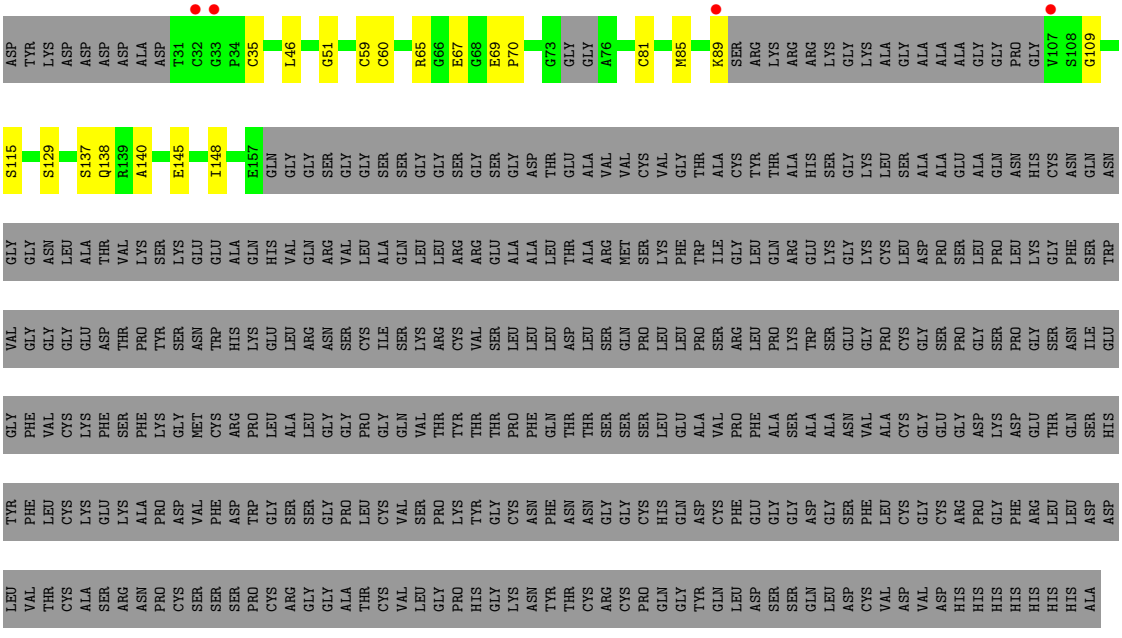
• Molecule 1: Insulin-like growth factor-binding protein 7,Complement component C1q receptor

Chain C:



• Molecule 1: Insulin-like growth factor-binding protein 7,Complement component C1q receptor

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	131.51Å 208.90Å 77.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 3.24 19.95 – 3.24	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.95-3.24) 99.8 (19.95-3.24)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 3.22Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.244 , 0.302 0.248 , 0.301	Depositor DCC
R_{free} test set	849 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	118.4	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 93.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5380	wwPDB-VP
Average B, all atoms (Å^2)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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	0.25	0/2010	0.45	0/2741
1	B	0.26	0/1963	0.46	0/2669
1	C	0.26	0/779	0.50	0/1053
1	D	0.25	0/730	0.48	0/987
All	All	0.25	0/5482	0.47	0/7450

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	1961	0	1776	22	0
1	B	1917	0	1727	27	0
1	C	766	0	705	12	0
1	D	719	0	655	12	0
2	A	7	0	0	0	0
2	B	5	0	0	0	0
2	C	3	0	0	0	0
2	D	2	0	0	0	0
All	All	5380	0	4863	69	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 7.

All (69) 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:27:GLU:HG3	1:A:207:THR:HG23	1.57	0.83
1:A:291:PHE:HA	1:A:302:SER:HA	1.62	0.80
1:B:73:GLN:HG3	1:B:158:PRO:HD3	1.69	0.73
1:C:140:ALA:HB1	1:C:145:GLU:HB2	1.72	0.69
1:A:287:CYS:HB3	1:A:291:PHE:HB2	1.77	0.67
1:D:81:CYS:HB3	1:D:85:MET:HB2	1.77	0.65
1:C:81:CYS:HB3	1:C:85:MET:HB2	1.78	0.65
1:A:199:VAL:HG22	1:A:223:VAL:HG13	1.85	0.58
1:B:274:ASP:N	1:B:274:ASP:OD1	2.39	0.56
1:B:293:LEU:HD23	1:C:54:ARG:HG2	1.87	0.55
1:B:30:VAL:HB	1:B:75:VAL:HG22	1.88	0.55
1:B:97:LEU:HG	1:B:114:PHE:HB3	1.89	0.54
1:C:119:VAL:HB	1:C:150:GLN:HG3	1.90	0.53
1:A:272:HIS:HB2	1:A:299:THR:HA	1.90	0.53
1:C:74:GLY:HA2	1:C:78:ARG:HH21	1.73	0.53
1:B:61:ALA:HA	1:B:181:LYS:HB2	1.91	0.53
1:D:46:LEU:H	1:D:46:LEU:HD23	1.72	0.53
1:B:37:TYR:OH	1:B:68:GLU:OE2	2.27	0.52
1:B:105:LEU:HD12	1:B:134:ASN:HA	1.92	0.52
1:A:104:CYS:N	1:A:136:CYS:HB3	2.25	0.51
1:A:260:PRO:HA	1:A:281:GLY:HA3	1.93	0.51
1:B:199:VAL:HG22	1:B:223:VAL:HG13	1.92	0.51
1:B:73:GLN:NE2	1:B:153:LEU:O	2.43	0.51
1:B:71:HIS:O	1:B:75:VAL:HG23	2.11	0.50
1:D:65:ARG:HB3	1:D:69:GLU:HB2	1.92	0.50
1:D:67:GLU:HG2	1:D:85:MET:HE1	1.94	0.49
1:A:205:PHE:CD2	1:A:207:THR:HB	2.48	0.49
1:C:71:CYS:HB3	1:C:111:CYS:SG	2.53	0.49
1:B:104:CYS:HA	1:B:136:CYS:HB3	1.96	0.48
1:B:121:GLU:OE1	1:B:121:GLU:N	2.48	0.47
1:C:104:GLY:O	1:C:107:VAL:HG12	2.15	0.47
1:D:140:ALA:O	1:D:145:GLU:N	2.48	0.47
1:A:37:TYR:OH	1:A:68:GLU:OE2	2.32	0.47
1:A:244:ALA:HB3	1:A:247:VAL:HB	1.97	0.46
1:D:137:SER:HA	1:D:148:ILE:HD12	1.97	0.46
1:A:111:LEU:HD12	1:A:122:ASP:HA	1.96	0.46
1:B:202:THR:HA	1:B:208:THR:HG22	1.98	0.46
1:A:276:PHE:HZ	1:D:51:GLY:HA3	1.80	0.46
1:B:29:VAL:HB	1:B:207:THR:HG21	1.97	0.46
1:D:115:SER:O	1:D:129:SER:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLY:O	1:B:187:MET:HG3	2.15	0.45
1:B:30:VAL:HG21	1:B:74:ARG:HD2	1.99	0.45
1:B:287:CYS:HB3	1:B:291:PHE:HB2	1.98	0.45
1:A:50:GLN:NE2	1:A:59:ASN:OD1	2.50	0.44
1:B:73:GLN:HG2	1:B:152:LEU:HD13	1.98	0.44
1:A:92:LYS:HB3	1:A:175:ILE:HD13	1.99	0.44
1:A:90:MET:O	1:A:174:ASN:HB3	2.18	0.44
1:D:65:ARG:NH1	1:D:70:PRO:O	2.51	0.44
1:C:46:LEU:H	1:C:46:LEU:HD23	1.83	0.43
1:B:292:ARG:HB3	1:B:303:ARG:NH1	2.33	0.43
1:B:44:LEU:HB3	1:B:48:GLU:HB2	2.01	0.43
1:B:140:ARG:HH22	1:B:163:GLY:HA2	1.83	0.42
1:D:59:CYS:SG	1:D:60:CYS:N	2.92	0.42
1:C:134:ARG:O	1:C:138:GLN:NE2	2.47	0.42
1:A:33:GLY:O	1:A:187:MET:HG3	2.19	0.42
1:D:89:LYS:HG2	1:D:109:GLY:HA3	2.02	0.42
1:A:273:GLN:OE1	1:A:288:ARG:HG3	2.18	0.42
1:B:92:LYS:HA	1:B:144:LEU:O	2.20	0.42
1:B:276:PHE:HB2	1:B:284:LEU:O	2.20	0.42
1:A:32:VAL:HG21	1:A:74:ARG:HH22	1.85	0.41
1:A:276:PHE:CZ	1:D:51:GLY:HA3	2.55	0.41
1:A:204:PRO:HD3	1:A:219:SER:OG	2.20	0.41
1:A:72:VAL:HG13	1:A:179:VAL:HG11	2.01	0.41
1:B:27:GLU:HG3	1:B:207:THR:HG23	2.03	0.41
1:B:303:ARG:NH1	1:C:52:GLU:OE1	2.54	0.41
1:B:128:TRP:HZ3	1:B:162:GLU:HB3	1.86	0.40
1:C:66:GLY:O	1:C:69:GLU:HB2	2.21	0.40
1:A:109:LEU:HD23	1:A:109:LEU:HA	1.98	0.40
1:C:66:GLY:O	1:C:111:CYS:HB2	2.21	0.40

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	270/481 (56%)	253 (94%)	17 (6%)	0	100 100
1	B	259/481 (54%)	245 (95%)	14 (5%)	0	100 100
1	C	111/481 (23%)	109 (98%)	1 (1%)	1 (1%)	17 52
1	D	102/481 (21%)	98 (96%)	4 (4%)	0	100 100
All	All	742/1924 (39%)	705 (95%)	36 (5%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	60	CYS

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	203/377 (54%)	201 (99%)	2 (1%)	76 88
1	B	197/377 (52%)	189 (96%)	8 (4%)	30 63
1	C	81/377 (22%)	81 (100%)	0	100 100
1	D	77/377 (20%)	75 (97%)	2 (3%)	46 74
All	All	558/1508 (37%)	546 (98%)	12 (2%)	52 76

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	CYS
1	A	136	CYS
1	B	73	GLN
1	B	136	CYS
1	B	140	ARG
1	B	149	SER
1	B	232	GLU
1	B	274	ASP
1	B	275	CYS
1	B	280	ASP

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Mol	Chain	Res	Type
1	D	35	CYS
1	D	138	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	59	ASN
1	B	50	GLN
1	B	54	ASN
1	B	59	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 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	274/481 (56%)	0.12	7 (2%)	56	44	102, 139, 190, 234	0
1	B	267/481 (55%)	0.40	14 (5%)	27	17	88, 149, 204, 232	0
1	C	115/481 (23%)	-0.07	1 (0%)	84	78	85, 111, 150, 212	0
1	D	108/481 (22%)	0.27	4 (3%)	41	30	117, 156, 202, 244	0
All	All	764/1924 (39%)	0.21	26 (3%)	45	33	85, 141, 198, 244	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	GLY	6.1
1	D	32	CYS	5.4
1	B	108	SER	4.2
1	B	26	THR	3.4
1	A	138	SER	3.4
1	A	237	TYR	3.4
1	D	33	GLY	3.2
1	C	32	CYS	3.1
1	B	134	ASN	3.1
1	D	89	LYS	2.8
1	B	135	SER	2.6
1	A	96	GLY	2.6
1	B	185	LYS	2.5
1	B	206	GLN	2.5
1	A	302	SER	2.4
1	B	143	SER	2.4
1	B	117	VAL	2.3
1	A	235	SER	2.2
1	A	95	ILE	2.2
1	B	119	GLY	2.2
1	B	150	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	38	THR	2.1
1	B	180	CYS	2.1
1	B	145	LEU	2.1
1	A	277	GLU	2.1
1	D	107	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.