Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 02:18 PM EDT

PDB ID	:	3OED
Title	:	The structure of the complex between complement receptor CR2 and its ligand complement fragment C3d
Authors	:	Isenman, D.E.; van den Elsen, J.M.H.
Deposited on	:	2010-08-12
Resolution	:	3.16 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 (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:

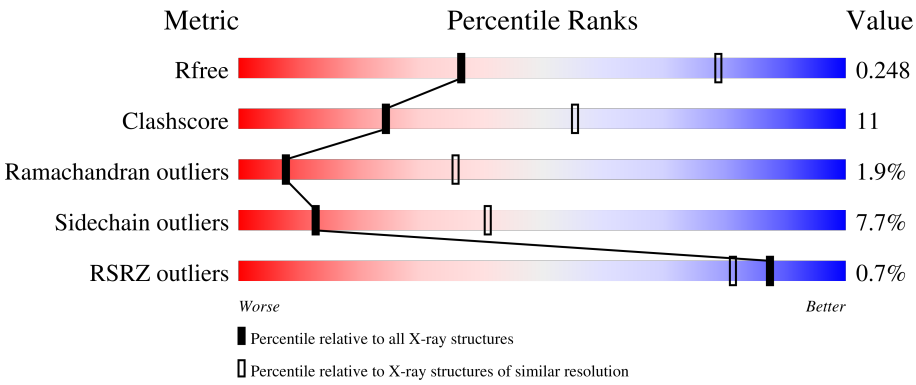
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.16 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	310	65% 29% • 5%
1	B	310	66% 26% • 5%
2	C	135	72% 24% • •
2	D	135	4% 68% 24% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6628 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 Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	294	2316	1490	388	428	10	0	0	0
1	B	294	2316	1490	388	428	10	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P01024
A	2	LEU	-	expression tag	UNP P01024
A	17	ALA	CYS	engineered mutation	UNP P01024
B	1	MET	-	expression tag	UNP P01024
B	2	LEU	-	expression tag	UNP P01024
B	17	ALA	CYS	engineered mutation	UNP P01024

- Molecule 2 is a protein called Complement receptor type 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	130	990	627	170	183	10	0	0	0
2	D	130	990	627	170	183	10	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	initiating methionine	UNP P20023
D	-1	MET	-	initiating methionine	UNP P20023

- Molecule 3 is water.

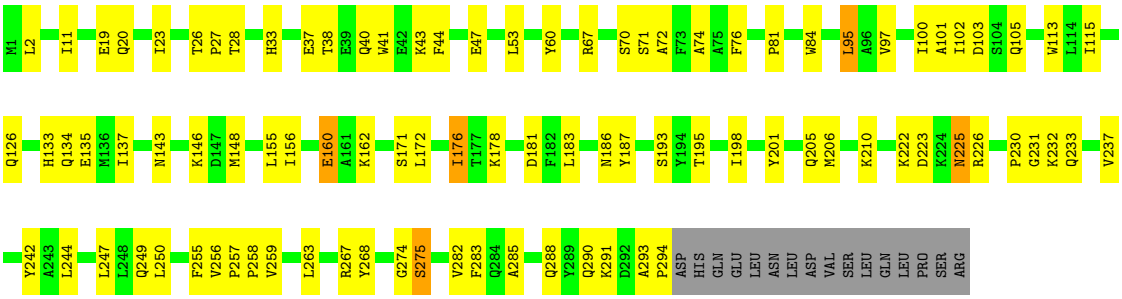
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	3	3	3	0	0
			Total	O		
3	C	4	4	4	0	0
			Total	O		
3	B	7	7	7	0	0
			Total	O		
3	D	2	2	2	0	0

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.

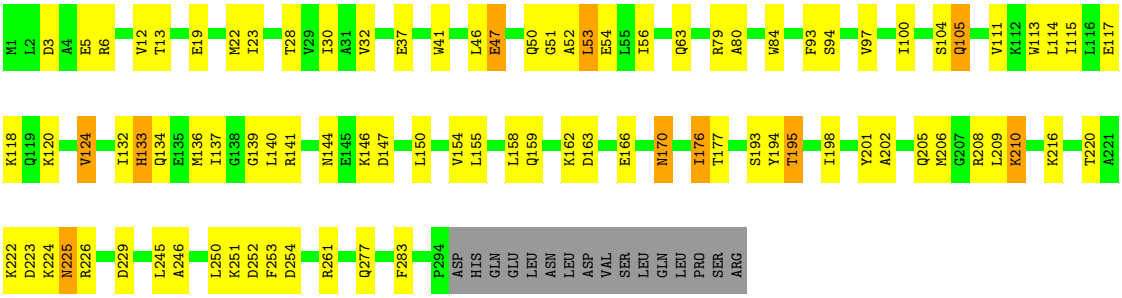
- Molecule 1: Complement C3

Chain A:



- Molecule 1: Complement C3

Chain B:

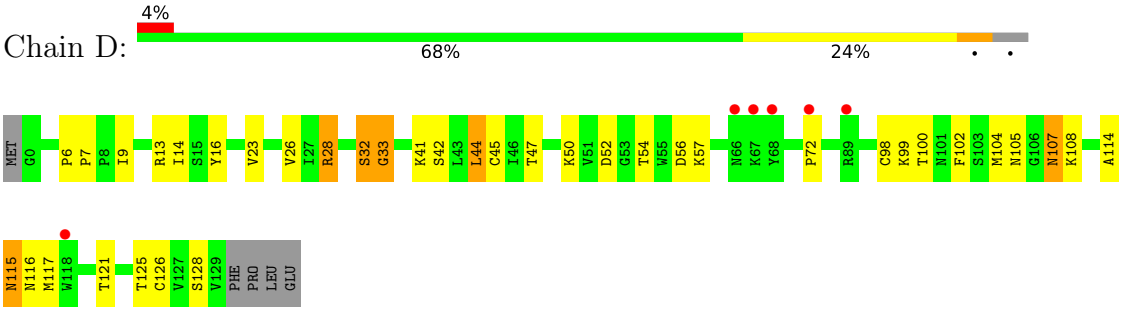


- Molecule 2: Complement receptor type 2

Chain C:

- Molecule 2: Complement receptor type 2

Chain D:


4%
68%
24%
MET G0 P6 P7 P8 I9 R13 I14 S15 Y16 V23 V26 I27 R28 S32 G33 K41 S42 L43 L44 C45 I46 T47 K50 V51 D52 G53 T54 W55 D56 K57 N66 K67 Y68 P72 R89 C98 K99 T100 N101 F102 S103 M104 N105 G106 N107 K108 A114
N115 N116 M117 W118 T121 T125 C126 V127 S128 V129 PHE PRO LEU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	146.12Å 146.12Å 253.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.00 – 3.16 47.00 – 3.16	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.00-3.16) 100.0 (47.00-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.189 , 0.259 0.184 , 0.248	Depositor DCC
R_{free} test set	919 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	74.3	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6628	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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 (i)

5.1 Standard geometry (i)

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	0.62	0/2365	0.70	0/3204
1	B	0.58	0/2365	0.67	0/3204
2	C	0.63	0/1019	0.73	1/1386 (0.1%)
2	D	0.55	0/1019	0.71	2/1386 (0.1%)
All	All	0.60	0/6768	0.70	3/9180 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	52	ASP	CB-CG-OD1	7.35	124.92	118.30
2	D	44	LEU	CA-CB-CG	6.61	130.50	115.30
2	C	52	ASP	CB-CG-OD1	5.73	123.46	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2316	0	2329	55	0
1	B	2316	0	2329	58	0
2	C	990	0	967	17	0
2	D	990	0	967	22	0
3	A	3	0	0	1	0
3	B	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	4	0	0	0	0
3	D	2	0	0	0	0
All	All	6628	0	6592	145	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 11.

All (145) 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:B:155:LEU:HD23	1:B:202:ALA:HB1	1.52	0.89
1:A:176:ILE:HG23	1:A:206:MET:HE2	1.57	0.87
1:A:225:ASN:HD21	1:A:226:ARG:HH11	1.21	0.84
2:D:102:PHE:HB3	2:D:126:CYS:HB3	1.63	0.80
1:A:148:MET:SD	1:A:186:ASN:HB2	2.24	0.77
1:A:2:LEU:HD12	1:A:283:PHE:CE1	2.22	0.74
1:A:233:GLN:O	1:A:237:VAL:HG23	1.87	0.74
1:A:249:GLN:HE22	2:C:83:ARG:HH21	1.37	0.73
1:A:41:TRP:HB2	3:A:312:HOH:O	1.95	0.66
1:B:170:ASN:HD22	1:B:170:ASN:H	1.43	0.66
1:A:37:GLU:OE1	1:A:291:LYS:HG2	1.96	0.65
1:A:19:GLU:OE1	1:A:133:HIS:HD2	1.79	0.65
1:B:208:ARG:HA	1:B:210:LYS:HE3	1.80	0.62
2:D:115:ASN:OD1	2:D:117:MET:HB2	1.98	0.62
1:A:143:ASN:O	1:A:146:LYS:HB3	2.00	0.62
2:C:28:ARG:HD3	2:C:41:LYS:HD2	1.81	0.61
1:B:84:TRP:CZ2	1:B:137:ILE:HA	2.36	0.60
2:C:100:THR:HG22	2:C:101:ASN:OD1	2.01	0.60
1:A:225:ASN:HD21	1:A:226:ARG:NH1	1.97	0.59
1:B:52:ALA:O	1:B:56:ILE:HG13	2.03	0.59
1:A:2:LEU:HD12	1:A:283:PHE:HE1	1.68	0.58
1:A:223:ASP:HB2	1:A:226:ARG:NH1	2.19	0.58
1:B:94:SER:O	1:B:97:VAL:HG12	2.03	0.58
1:A:223:ASP:HB2	1:A:226:ARG:HH12	1.68	0.57
1:B:111:VAL:HG13	1:B:158:LEU:HD22	1.85	0.57
1:A:102:ILE:HG22	1:A:103:ASP:N	2.20	0.57
1:B:51:GLY:HA2	1:B:54:GLU:OE1	2.05	0.56
1:A:257:PRO:HD2	1:A:258:PRO:HD2	1.86	0.56
1:B:225:ASN:ND2	1:B:226:ARG:HG2	2.20	0.56
2:D:114:ALA:C	2:D:116:ASN:H	2.09	0.56
2:D:23:VAL:HA	2:D:45:CYS:SG	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:ARG:HD3	2:D:41:LYS:HD3	1.88	0.55
1:B:209:LEU:HD23	1:B:250:LEU:HD11	1.89	0.55
1:B:30:ILE:HG12	1:B:283:PHE:HB2	1.89	0.55
1:B:104:SER:HB3	2:D:26:VAL:CG2	2.37	0.54
2:D:56:ASP:OD1	2:D:57:LYS:HG2	2.07	0.54
1:B:23:ILE:HG13	1:B:136:MET:CE	2.37	0.54
1:B:176:ILE:HG23	1:B:206:MET:CE	2.38	0.54
1:A:38:THR:HG22	1:A:290:GLN:HG3	1.88	0.54
1:B:225:ASN:HD21	1:B:226:ARG:NH1	2.06	0.54
1:A:222:LYS:O	1:A:223:ASP:HB2	2.08	0.53
1:A:11:ILE:HA	1:A:28:THR:HG23	1.89	0.53
1:B:28:THR:O	1:B:32:VAL:HG23	2.09	0.53
1:B:139:GLY:HA3	1:B:194:TYR:CE1	2.44	0.53
2:D:47:THR:O	2:D:47:THR:HG23	2.07	0.53
1:B:170:ASN:H	1:B:170:ASN:ND2	2.06	0.52
1:A:19:GLU:OE1	1:A:133:HIS:CD2	2.62	0.52
1:A:44:PHE:O	1:A:44:PHE:CG	2.63	0.52
1:B:137:ILE:HD11	1:B:141:ARG:HA	1.92	0.52
1:A:155:LEU:HD21	1:A:206:MET:HE1	1.90	0.52
2:D:99:LYS:HB3	2:D:102:PHE:CD1	2.44	0.52
1:B:176:ILE:HG22	1:B:177:THR:N	2.26	0.51
1:A:201:TYR:OH	1:A:205:GLN:NE2	2.43	0.51
2:C:42:SER:O	2:C:43:LEU:HD12	2.11	0.51
2:C:7:PRO:HB2	2:C:59:ALA:HB2	1.93	0.51
1:A:84:TRP:CZ2	1:A:137:ILE:HA	2.46	0.50
1:B:208:ARG:HA	1:B:210:LYS:CE	2.40	0.50
1:A:183:LEU:O	1:A:187:TYR:HB2	2.12	0.50
1:B:97:VAL:HA	1:B:100:ILE:O	2.11	0.50
2:D:99:LYS:HB3	2:D:102:PHE:HD1	1.75	0.50
2:D:107:ASN:HD22	2:D:108:LYS:N	2.09	0.50
1:A:60:TYR:CE1	1:A:102:ILE:HG23	2.47	0.50
1:B:193:SER:HB2	1:B:229:ASP:OD1	2.12	0.50
1:A:84:TRP:CD2	1:A:137:ILE:HG22	2.47	0.49
1:A:288:GLN:HE22	1:A:291:LYS:NZ	2.10	0.49
1:B:225:ASN:HD21	1:B:226:ARG:HH11	1.60	0.49
2:C:84:GLY:HA3	2:C:94:VAL:HG22	1.95	0.49
1:B:23:ILE:HG13	1:B:136:MET:HE1	1.94	0.49
1:B:201:TYR:HA	1:B:246:ALA:HB2	1.95	0.49
1:A:84:TRP:CE2	1:A:137:ILE:HG22	2.47	0.49
2:C:37:LEU:HD11	2:C:60:PRO:HB2	1.95	0.49
1:B:159:GLN:NE2	1:B:205:GLN:OE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:81:LYS:HG3	2:C:94:VAL:HG13	1.95	0.48
2:D:98:CYS:SG	2:D:104:MET:HB2	2.53	0.48
1:A:74:ALA:HB2	1:A:81:PRO:HA	1.95	0.48
1:A:198:ILE:HD12	1:A:242:TYR:CE2	2.48	0.48
2:D:107:ASN:HD22	2:D:108:LYS:H	1.61	0.48
1:A:26:THR:N	1:A:27:PRO:HD2	2.29	0.48
2:D:114:ALA:O	2:D:116:ASN:N	2.47	0.48
1:A:156:ILE:O	1:A:160:GLU:HB2	2.14	0.47
1:B:113:TRP:CD1	1:B:117:GLU:HG3	2.49	0.47
1:B:146:LYS:HG3	1:B:147:ASP:N	2.30	0.47
1:A:101:ALA:HB2	2:C:17:TYR:HB3	1.96	0.47
1:B:195:THR:HA	1:B:198:ILE:HG22	1.97	0.47
1:A:33:HIS:CD2	1:A:95:LEU:HD11	2.50	0.46
1:B:47:GLU:H	1:B:47:GLU:HG3	1.36	0.46
1:A:244:LEU:HD23	1:A:285:ALA:HB1	1.97	0.46
1:B:176:ILE:HG23	1:B:206:MET:HE1	1.98	0.46
1:B:132:ILE:O	1:B:134:GLN:N	2.48	0.46
2:C:89:ARG:HD2	2:C:89:ARG:HA	1.82	0.46
1:B:136:MET:O	1:B:277:GLN:HG2	2.16	0.45
1:A:72:ALA:HB2	1:A:113:TRP:CD2	2.51	0.45
2:C:99:LYS:O	2:C:100:THR:C	2.55	0.45
1:A:70:SER:O	1:A:71:SER:HB2	2.16	0.45
2:C:28:ARG:NH1	2:C:42:SER:OG	2.50	0.45
1:B:150:LEU:O	1:B:154:VAL:HG23	2.17	0.45
1:B:113:TRP:CH2	1:B:118:LYS:HE2	2.52	0.45
1:A:255:PHE:O	1:A:255:PHE:CD1	2.69	0.44
1:A:263:LEU:HD22	1:A:282:VAL:HG23	1.98	0.44
1:B:84:TRP:HE1	1:B:140:LEU:HD13	1.81	0.44
1:B:113:TRP:CZ2	1:B:118:LYS:HE2	2.53	0.44
1:B:46:LEU:HD12	1:B:46:LEU:O	2.18	0.44
1:A:97:VAL:HA	1:A:100:ILE:O	2.16	0.44
1:A:268:TYR:OH	1:A:275:SER:HB2	2.17	0.44
1:B:12:VAL:HG12	1:B:13:THR:N	2.33	0.44
2:C:98:CYS:HB3	2:C:102:PHE:HB2	1.98	0.44
2:D:28:ARG:NH1	2:D:42:SER:OG	2.51	0.44
1:A:134:GLN:O	1:A:137:ILE:HG12	2.17	0.43
1:A:257:PRO:CD	1:A:258:PRO:HD2	2.46	0.43
1:B:93:PHE:N	1:B:93:PHE:CD1	2.85	0.43
1:B:216:LYS:O	1:B:220:THR:OG1	2.32	0.43
1:B:111:VAL:HA	1:B:114:LEU:HD12	2.01	0.43
2:D:9:ILE:HG22	2:D:14:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:GLN:H	1:B:105:GLN:HG2	1.70	0.43
2:D:32:SER:OG	2:D:33:GLY:N	2.52	0.43
1:A:135:GLU:O	1:A:274:GLY:HA2	2.19	0.42
1:A:115:ILE:HG21	1:A:171:SER:OG	2.19	0.42
1:B:23:ILE:HG13	1:B:136:MET:HE3	2.01	0.42
1:A:293:ALA:HA	1:A:294:PRO:HD3	1.91	0.42
1:B:19:GLU:OE1	1:B:133:HIS:HD2	2.02	0.42
2:D:6:PRO:HA	2:D:7:PRO:HD2	1.84	0.42
1:A:222:LYS:HD3	1:A:226:ARG:NH2	2.34	0.42
1:A:256:VAL:O	1:A:259:VAL:HB	2.19	0.42
1:A:288:GLN:NE2	1:A:291:LYS:NZ	2.67	0.42
2:C:54:THR:HG21	2:D:54:THR:HG21	2.01	0.42
1:B:53:LEU:HD12	2:D:16:TYR:CB	2.49	0.42
1:B:201:TYR:CA	1:B:246:ALA:HB2	2.49	0.42
1:A:162:LYS:HA	1:A:172:LEU:HD21	2.02	0.42
1:B:251:LYS:O	1:B:253:PHE:N	2.52	0.42
1:A:288:GLN:HE22	1:A:291:LYS:HZ2	1.68	0.41
1:B:22:MET:HG2	1:B:63:GLN:OE1	2.20	0.41
1:A:19:GLU:O	1:A:23:ILE:HG13	2.19	0.41
1:A:205:GLN:HA	1:A:249:GLN:HG2	2.02	0.41
1:B:176:ILE:HG23	1:B:206:MET:HE2	2.02	0.41
1:A:247:LEU:HA	1:A:250:LEU:HD12	2.03	0.41
1:B:79:ARG:HG2	1:B:80:ALA:N	2.35	0.41
2:C:66:ASN:OD1	2:C:66:ASN:C	2.59	0.41
1:B:37:GLU:OE2	2:D:13:ARG:NH2	2.54	0.41
2:C:102:PHE:HA	2:C:127:VAL:O	2.21	0.41
1:B:32:VAL:HG13	1:B:41:TRP:HZ2	1.86	0.41
1:B:53:LEU:HD12	2:D:16:TYR:HB2	2.02	0.41
1:B:170:ASN:ND2	1:B:170:ASN:N	2.68	0.41
1:B:120:LYS:HD2	1:B:124:VAL:HG12	2.03	0.40
1:B:201:TYR:CE1	1:B:245:LEU:HB3	2.57	0.40
2:C:98:CYS:SG	2:C:104:MET:HB2	2.62	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	292/310 (94%)	266 (91%)	22 (8%)	4 (1%)	11	43
1	B	292/310 (94%)	261 (89%)	24 (8%)	7 (2%)	6	30
2	C	128/135 (95%)	116 (91%)	10 (8%)	2 (2%)	9	40
2	D	128/135 (95%)	115 (90%)	10 (8%)	3 (2%)	6	31
All	All	840/890 (94%)	758 (90%)	66 (8%)	16 (2%)	8	36

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	PRO
2	D	72	PRO
1	A	181	ASP
1	A	231	GLY
1	B	163	ASP
2	D	33	GLY
2	D	115	ASN
1	A	40	GLN
1	B	133	HIS
1	B	224	LYS
2	C	82	ILE
1	B	166	GLU
2	C	33	GLY
1	B	162	LYS
1	B	252	ASP
1	B	115	ILE

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	243/259 (94%)	224 (92%)	19 (8%)	12	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	243/259 (94%)	225 (93%)	18 (7%)	13	43
2	C	112/118 (95%)	104 (93%)	8 (7%)	14	44
2	D	112/118 (95%)	102 (91%)	10 (9%)	9	33
All	All	710/754 (94%)	655 (92%)	55 (8%)	13	41

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	43	LYS
1	A	47	GLU
1	A	53	LEU
1	A	67	ARG
1	A	76	PHE
1	A	95	LEU
1	A	105	GLN
1	A	126	GLN
1	A	160	GLU
1	A	176	ILE
1	A	178	LYS
1	A	193	SER
1	A	195	THR
1	A	210	LYS
1	A	225	ASN
1	A	232	LYS
1	A	267	ARG
1	A	275	SER
2	C	15	SER
2	C	26	VAL
2	C	30	SER
2	C	32	SER
2	C	41	LYS
2	C	61	LYS
2	C	69	SER
2	C	70	SER
1	B	3	ASP
1	B	5	GLU
1	B	6	ARG
1	B	47	GLU
1	B	50	GLN
1	B	53	LEU

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Mol	Chain	Res	Type
1	B	105	GLN
1	B	124	VAL
1	B	144	ASN
1	B	170	ASN
1	B	176	ILE
1	B	195	THR
1	B	210	LYS
1	B	222	LYS
1	B	223	ASP
1	B	225	ASN
1	B	254	ASP
1	B	261	ARG
2	D	28	ARG
2	D	32	SER
2	D	44	LEU
2	D	50	LYS
2	D	100	THR
2	D	105	ASN
2	D	107	ASN
2	D	121	THR
2	D	125	THR
2	D	128	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	62	GLN
1	A	133	HIS
1	A	143	ASN
1	A	189	ASN
1	A	205	GLN
1	A	225	ASN
1	A	249	GLN
1	A	288	GLN
1	B	133	HIS
1	B	143	ASN
1	B	159	GLN
1	B	170	ASN
1	B	189	ASN
1	B	225	ASN
1	B	266	GLN

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Mol	Chain	Res	Type
2	D	11	ASN
2	D	66	ASN
2	D	90	HIS
2	D	107	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	294/310 (94%)	-0.30	0	100	100	40, 68, 92, 102	0
1	B	294/310 (94%)	-0.20	0	100	100	52, 76, 101, 111	0
2	C	130/135 (96%)	-0.23	0	100	100	55, 71, 84, 91	0
2	D	130/135 (96%)	0.18	6 (4%)	32	18	59, 109, 138, 146	0
All	All	848/890 (95%)	-0.18	6 (0%)	87	81	40, 73, 124, 146	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	89	ARG	3.0
2	D	67	LYS	2.7
2	D	68	TYR	2.3
2	D	72	PRO	2.2
2	D	66	ASN	2.1
2	D	118	TRP	2.0

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.