Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:50 PM GMT

PDB ID	:	1QSC
Title	:	CRYSTAL STRUCTURE OF THE TRAF DOMAIN OF TRAF2 IN A COMPLEX WITH A PEPTIDE FROM THE CD40 RECEPTOR
Authors	:	McWhirter, S.M.; Pullen, S.S.; Holton, J.M.; Crute, J.J.; Kehry, M.R.; Alber, T.
Deposited on	:	1999-06-20
Resolution	:	2.40 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 (i) symbol.

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

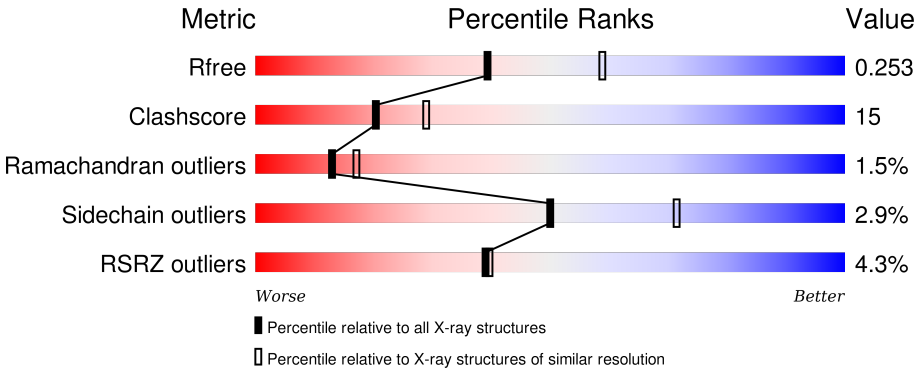
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	191	5%, 71%, 20%, 6%
1	B	191	3%, 74%, 18%, 6%
1	C	191	3%, 71%, 21%, 6%
2	D	7	86%, 14%
2	E	7	14%, 57%, 43%

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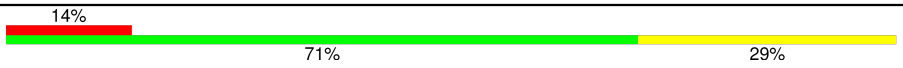
Mol	Chain	Length	Quality of chain
2	F	7	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4589 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 TNF RECEPTOR ASSOCIATED FACTOR 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	Se	0	0	0
			1380	881	236	253	3	7			
1	B	179	Total	C	N	O	S	Se	0	0	0
			1377	880	232	255	3	7			
1	C	179	Total	C	N	O	S	Se	0	0	0
			1394	891	242	251	3	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	ALA	PRO	CONFLICT	UNP Q12933
A	365	ARG	LEU	CONFLICT	UNP Q12933
B	362	ALA	PRO	CONFLICT	UNP Q12933
B	365	ARG	LEU	CONFLICT	UNP Q12933
C	362	ALA	PRO	CONFLICT	UNP Q12933
C	365	ARG	LEU	CONFLICT	UNP Q12933

- Molecule 2 is a protein called CD40 RECEPTOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	7	Total	C	N	O	0	0	0
			55	36	7	12			
2	E	7	Total	C	N	O	0	0	0
			55	36	7	12			
2	F	7	Total	C	N	O	0	0	0
			55	36	7	12			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	101	Total	O	0	0
			101	101		

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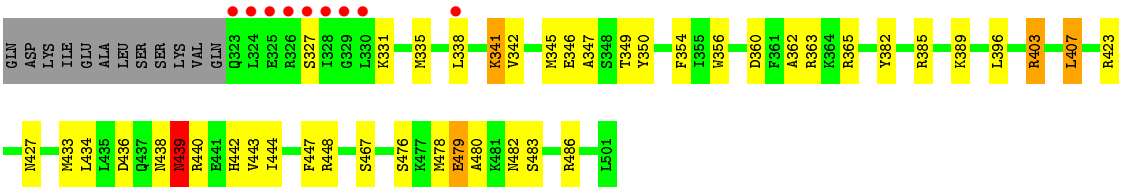
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	75	Total O 75 75	0	0
3	C	78	Total O 78 78	0	0
3	D	10	Total O 10 10	0	0
3	E	5	Total O 5 5	0	0
3	F	4	Total O 4 4	0	0

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.

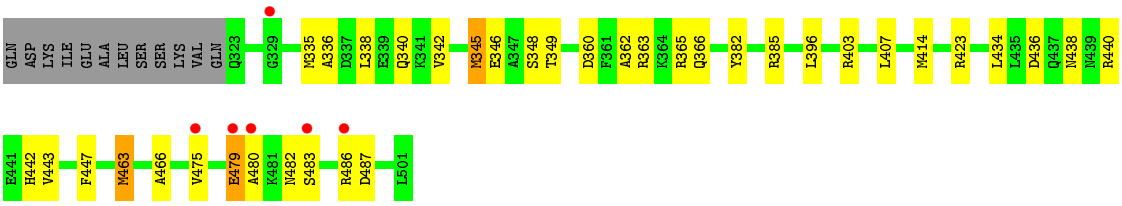
- Molecule 1: TNF RECEPTOR ASSOCIATED FACTOR 2

Chain A:



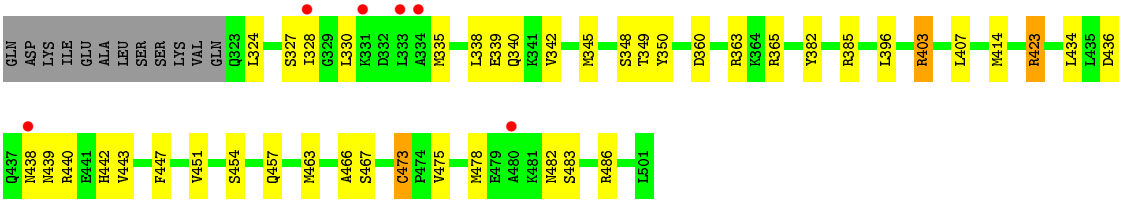
- Molecule 1: TNF RECEPTOR ASSOCIATED FACTOR 2

Chain B:



- Molecule 1: TNF RECEPTOR ASSOCIATED FACTOR 2

Chain C:

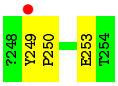


- Molecule 2: CD40 RECEPTOR

Chain D:

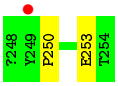
- Molecule 2: CD40 RECEPTOR

Chain E:



- Molecule 2: CD40 RECEPTOR

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	87.11Å 90.09Å 92.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40 64.58 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (25.00-2.40) 98.4 (64.58-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	4.46 (at 2.40Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.215 , 0.257 0.211 , 0.253	Depositor DCC
R_{free} test set	1476 reflections (5.13%)	DCC
Wilson B-factor (Å^2)	56.1	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 58.6	EDS
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 28844 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4589	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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, 0.375 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: ACE

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	0.49	0/1403	0.62	1/1889 (0.1%)
1	B	0.51	1/1400 (0.1%)	0.62	0/1887
1	C	0.50	0/1417	0.63	0/1906
2	D	0.38	0/54	0.59	0/74
2	E	0.37	0/54	0.63	0/74
2	F	0.44	0/54	0.62	0/74
All	All	0.50	1/4382 (0.0%)	0.62	1/5904 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	463	MSE	CG-SE	-5.50	1.76	1.95

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	407	LEU	N-CA-C	-5.10	97.23	111.00

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	1380	0	1339	57	0
1	B	1377	0	1330	40	0
1	C	1394	0	1375	44	0
2	D	55	0	51	3	0
2	E	55	0	51	4	0
2	F	55	0	51	3	0
3	A	101	0	0	4	0
3	B	75	0	0	1	0
3	C	78	0	0	4	0
3	D	10	0	0	0	0
3	E	5	0	0	0	0
3	F	4	0	0	0	0
All	All	4589	0	4197	124	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 15.

All (124) 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:335:MSE:HG2	1:B:335:MSE:HE1	1.44	0.98
1:A:342:VAL:HG13	1:C:345:MSE:HE1	1.45	0.97
1:A:436:ASP:H	1:A:442:HIS:CD2	1.84	0.94
1:A:436:ASP:H	1:A:442:HIS:HD2	1.00	0.93
1:B:438:ASN:HD22	1:B:483:SER:HB3	1.35	0.89
1:A:438:ASN:HD22	1:A:483:SER:HB3	1.38	0.89
1:B:436:ASP:H	1:B:442:HIS:CD2	1.91	0.88
1:A:345:MSE:HE1	1:B:345:MSE:HB3	1.56	0.86
1:C:436:ASP:H	1:C:442:HIS:HD2	1.23	0.85
1:B:436:ASP:H	1:B:442:HIS:HD2	1.24	0.84
1:A:403:ARG:HH11	1:A:403:ARG:HG2	1.46	0.81
1:A:447:PHE:CD1	2:D:250:PRO:HG3	2.17	0.79
1:C:436:ASP:H	1:C:442:HIS:CD2	2.01	0.78
1:A:342:VAL:HG13	1:C:345:MSE:CE	2.15	0.76
1:B:438:ASN:HD22	1:B:483:SER:CB	2.03	0.71
1:B:447:PHE:CD1	2:E:250:PRO:HG3	2.25	0.71
1:A:338:LEU:HD22	1:C:338:LEU:HD11	1.72	0.71
1:C:438:ASN:HD22	1:C:483:SER:HB3	1.57	0.70
1:B:348:SER:HB3	3:B:113:HOH:O	1.95	0.67
1:A:335:MSE:CG	1:B:335:MSE:HE1	2.23	0.66
1:B:345:MSE:HE2	1:C:342:VAL:HG13	1.77	0.66
1:A:476:SER:O	1:A:479:GLU:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ASN:HD22	1:A:483:SER:CB	2.10	0.65
1:B:434:LEU:HB3	1:B:443:VAL:HB	1.77	0.64
1:A:436:ASP:N	1:A:442:HIS:HD2	1.84	0.63
1:B:362:ALA:O	1:B:366:GLN:HG3	2.00	0.61
1:A:341:LYS:NZ	1:A:341:LYS:HB2	2.15	0.61
1:C:447:PHE:CD1	2:F:250:PRO:HG3	2.35	0.61
1:A:403:ARG:NH1	1:A:403:ARG:HG2	2.16	0.60
1:A:434:LEU:HB3	1:A:443:VAL:HB	1.85	0.59
1:A:345:MSE:HE1	1:B:345:MSE:HE3	1.84	0.58
1:A:341:LYS:HD2	1:B:346:GLU:OE2	2.03	0.58
1:C:438:ASN:HD22	1:C:483:SER:CB	2.16	0.58
1:A:335:MSE:HG2	1:B:335:MSE:CE	2.29	0.58
1:A:438:ASN:CG	1:A:486:ARG:HH22	2.06	0.58
1:B:403:ARG:HG2	1:B:403:ARG:HH11	1.68	0.57
1:C:434:LEU:HB3	1:C:443:VAL:HB	1.85	0.57
1:A:360:ASP:OD2	1:A:363:ARG:HD2	2.04	0.56
1:B:396:LEU:HA	1:B:407:LEU:HD12	1.87	0.56
1:C:454:SER:O	1:C:457:GLN:HG2	2.06	0.56
1:A:396:LEU:HD23	1:A:407:LEU:HD11	1.87	0.56
1:A:327:SER:O	1:A:331:LYS:HD3	2.04	0.56
1:C:360:ASP:OD2	1:C:363:ARG:HD3	2.05	0.55
1:C:467:SER:OG	2:F:250:PRO:HB2	2.06	0.55
1:A:346:GLU:HG3	3:A:218:HOH:O	2.06	0.55
1:C:338:LEU:HD23	1:C:338:LEU:O	2.07	0.54
1:B:338:LEU:HD21	1:C:338:LEU:HD22	1.88	0.54
1:A:362:ALA:HB3	3:A:54:HOH:O	2.08	0.53
1:B:479:GLU:OE1	1:B:479:GLU:HA	2.09	0.53
1:C:324:LEU:O	1:C:328:ILE:HG12	2.08	0.52
1:C:451:VAL:HG22	3:C:89:HOH:O	2.09	0.52
1:C:385:ARG:HG3	1:C:385:ARG:HH11	1.73	0.52
1:A:467:SER:OG	2:D:250:PRO:HB2	2.10	0.52
1:C:365:ARG:HG2	1:C:365:ARG:HH11	1.74	0.52
1:A:396:LEU:HA	1:A:407:LEU:CD1	2.40	0.52
1:A:338:LEU:HD22	1:C:338:LEU:CD1	2.39	0.51
1:B:438:ASN:ND2	1:B:483:SER:HB3	2.16	0.51
1:A:345:MSE:CE	1:B:345:MSE:HE3	2.41	0.51
1:C:327:SER:O	1:C:330:LEU:HB3	2.10	0.50
1:A:365:ARG:HH11	1:A:365:ARG:HG2	1.75	0.50
1:A:396:LEU:HA	1:A:407:LEU:HD12	1.94	0.50
1:B:365:ARG:HG2	1:B:365:ARG:HH11	1.78	0.49
1:B:438:ASN:CG	1:B:486:ARG:HH22	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ARG:HG2	1:B:349:THR:HG22	1.94	0.48
1:C:396:LEU:HA	1:C:407:LEU:HD12	1.95	0.48
1:C:350:TYR:CD2	1:C:385:ARG:HA	2.48	0.48
1:A:382:TYR:CE2	1:A:389:LYS:HG3	2.49	0.47
1:B:466:ALA:HB3	2:E:253:GLU:CD	2.34	0.47
1:A:438:ASN:ND2	1:A:483:SER:HB3	2.18	0.47
1:C:403:ARG:HG2	1:C:403:ARG:HH11	1.78	0.47
1:A:338:LEU:HD21	1:B:342:VAL:HG21	1.97	0.47
1:C:365:ARG:NH2	1:C:475:VAL:HG22	2.29	0.47
1:B:396:LEU:HD23	1:B:407:LEU:HD11	1.96	0.47
1:C:438:ASN:CG	1:C:486:ARG:HH22	2.19	0.46
1:A:439:ASN:HA	1:A:439:ASN:HD22	1.54	0.46
1:C:385:ARG:HG3	1:C:385:ARG:NH1	2.31	0.46
1:C:436:ASP:OD1	1:C:438:ASN:HB2	2.16	0.46
1:A:403:ARG:CG	1:A:403:ARG:NH1	2.79	0.46
1:C:466:ALA:HB3	2:F:253:GLU:CD	2.36	0.46
1:B:385:ARG:HG2	1:C:349:THR:HG22	1.96	0.46
1:A:478:MSE:HA	1:A:482:ASN:ND2	2.30	0.46
1:A:335:MSE:SE	1:B:335:MSE:HE1	2.66	0.45
1:C:478:MSE:HA	1:C:482:ASN:ND2	2.31	0.45
1:A:385:ARG:HH11	1:A:385:ARG:HG3	1.82	0.45
1:A:448:ARG:HB3	3:A:182:HOH:O	2.16	0.45
1:A:447:PHE:CG	2:D:250:PRO:HG3	2.52	0.45
1:A:365:ARG:NH1	1:A:365:ARG:HG2	2.32	0.45
1:A:350:TYR:CD2	1:A:385:ARG:HA	2.52	0.45
1:C:365:ARG:HG2	1:C:365:ARG:NH1	2.32	0.44
1:B:414:MSE:HG2	1:B:463:MSE:HG2	1.98	0.44
1:A:338:LEU:O	1:A:338:LEU:HD23	2.18	0.44
1:B:403:ARG:HG2	1:B:403:ARG:NH1	2.33	0.44
1:B:360:ASP:OD2	1:B:363:ARG:NE	2.50	0.44
1:C:382:TYR:N	1:C:382:TYR:CD1	2.86	0.44
1:C:423:ARG:HG3	3:C:264:HOH:O	2.18	0.43
1:B:396:LEU:HA	1:B:407:LEU:CD1	2.48	0.43
1:A:382:TYR:CD1	1:A:382:TYR:N	2.86	0.43
1:B:365:ARG:NH2	1:B:475:VAL:HG22	2.33	0.43
1:C:342:VAL:HA	1:C:345:MSE:HE3	2.00	0.43
1:C:414:MSE:HG2	1:C:463:MSE:HG2	2.00	0.43
1:B:436:ASP:N	1:B:442:HIS:HD2	2.05	0.43
1:C:443:VAL:HG11	1:C:473:CYS:HB2	2.01	0.43
1:C:365:ARG:HH21	1:C:475:VAL:CG2	2.30	0.43
1:A:341:LYS:HZ2	1:A:341:LYS:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:ARG:NH2	1:C:475:VAL:CG2	2.82	0.42
1:A:342:VAL:O	1:A:346:GLU:HG2	2.19	0.42
1:B:447:PHE:CG	2:E:250:PRO:HG3	2.53	0.42
1:A:433:MSE:HE3	1:A:444:ILE:HD11	2.00	0.42
1:C:348:SER:HB3	3:C:153:HOH:O	2.20	0.42
1:C:340:GLN:HA	1:C:340:GLN:HE21	1.84	0.42
1:A:354:PHE:CE2	1:A:356:TRP:HB2	2.55	0.41
1:A:349:THR:HG22	1:C:385:ARG:HG2	2.02	0.41
1:A:396:LEU:HD23	1:A:407:LEU:CD1	2.51	0.41
1:C:335:MSE:O	1:C:339:GLU:HG3	2.20	0.41
1:A:447:PHE:C	1:A:447:PHE:CD1	2.94	0.41
1:A:433:MSE:HG2	1:A:444:ILE:HG12	2.02	0.41
2:E:249:TYR:HA	2:E:250:PRO:HD3	1.91	0.41
1:B:382:TYR:N	1:B:382:TYR:CD1	2.88	0.41
1:B:365:ARG:HG2	1:B:365:ARG:NH1	2.35	0.40
1:B:447:PHE:C	1:B:447:PHE:CD1	2.95	0.40
1:A:433:MSE:HE3	1:A:444:ILE:CD1	2.52	0.40
1:C:423:ARG:NH1	3:C:264:HOH:O	2.55	0.40
1:A:347:ALA:HA	3:A:16:HOH:O	2.20	0.40
1:B:336:ALA:O	1:B:340:GLN: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	177/191 (93%)	167 (94%)	6 (3%)	4 (2%)	8 8
1	B	177/191 (93%)	165 (93%)	9 (5%)	3 (2%)	11 14
1	C	177/191 (93%)	168 (95%)	8 (4%)	1 (1%)	30 43
2	D	5/7 (71%)	5 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	E	5/7 (71%)	5 (100%)	0	0	100 100
2	F	5/7 (71%)	5 (100%)	0	0	100 100
All	All	546/594 (92%)	515 (94%)	23 (4%)	8 (2%)	13 17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	440	ARG
1	A	479	GLU
1	A	480	ALA
1	B	480	ALA
1	A	439	ASN
1	B	479	GLU
1	C	439	ASN
1	A	440	ARG

5.3.2 Protein sidechains

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	144/158 (91%)	139 (96%)	5 (4%)	43 64
1	B	144/158 (91%)	140 (97%)	4 (3%)	51 72
1	C	147/158 (93%)	143 (97%)	4 (3%)	52 73
2	D	6/6 (100%)	6 (100%)	0	100 100
2	E	6/6 (100%)	6 (100%)	0	100 100
2	F	6/6 (100%)	6 (100%)	0	100 100
All	All	453/492 (92%)	440 (97%)	13 (3%)	50 71

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	341	LYS
1	A	403	ARG

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Mol	Chain	Res	Type
1	A	423	ARG
1	A	427	ASN
1	A	439	ASN
1	B	345	MSE
1	B	423	ARG
1	B	482	ASN
1	B	487	ASP
1	C	403	ARG
1	C	423	ARG
1	C	440	ARG
1	C	473	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	ASN
1	A	439	ASN
1	A	442	HIS
1	B	366	GLN
1	B	427	ASN
1	B	438	ASN
1	B	442	HIS
1	C	340	GLN
1	C	427	ASN
1	C	442	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 carbohydrates 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	172/191 (90%)	0.28	9 (5%) 31 31	33, 50, 118, 135	0
1	B	172/191 (90%)	0.24	6 (3%) 48 48	31, 54, 114, 130	0
1	C	172/191 (90%)	0.19	6 (3%) 48 48	31, 51, 117, 135	0
2	D	6/7 (85%)	-0.09	0 100 100	41, 43, 49, 55	0
2	E	6/7 (85%)	0.40	1 (16%) 2 2	53, 57, 64, 89	0
2	F	6/7 (85%)	0.70	1 (16%) 2 2	40, 47, 67, 92	0
All	All	534/594 (89%)	0.24	23 (4%) 39 40	31, 52, 118, 135	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	GLN	7.2
1	A	324	LEU	5.5
1	A	326	ARG	5.4
1	A	327	SER	4.4
1	A	330	LEU	4.2
1	A	328	ILE	4.1
1	B	483	SER	3.7
1	B	486	ARG	3.6
1	C	334	ALA	3.6
1	A	338	LEU	3.6
1	B	329	GLY	3.4
1	A	325	GLU	3.2
1	B	480	ALA	3.1
1	C	328	ILE	3.0
2	F	249	TYR	2.8
2	E	249	TYR	2.5
1	C	480	ALA	2.4
1	B	479	GLU	2.3
1	C	333	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	329	GLY	2.3
1	C	438	ASN	2.1
1	C	331	LYS	2.0
1	B	475	VAL	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 carbohydrates 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.