Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 09:12 PM GMT

PDB ID	:	4ZOM
Title	:	RORgamma in complex with inverse agonist 4j.
Authors	:	Marcotte, D.J.
Deposited on	:	2015-05-06
Resolution	:	2.27 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:

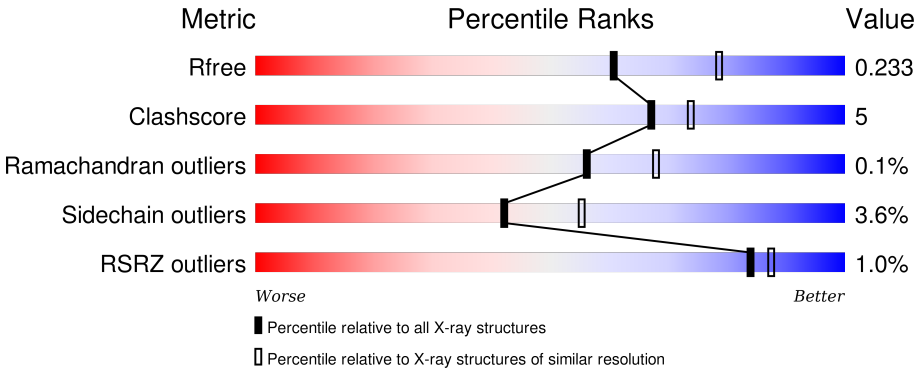
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.27 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	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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	225	71% 27%
1	B	225	71% 26%
1	C	225	74% 21%
1	D	225	72% 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7255 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.

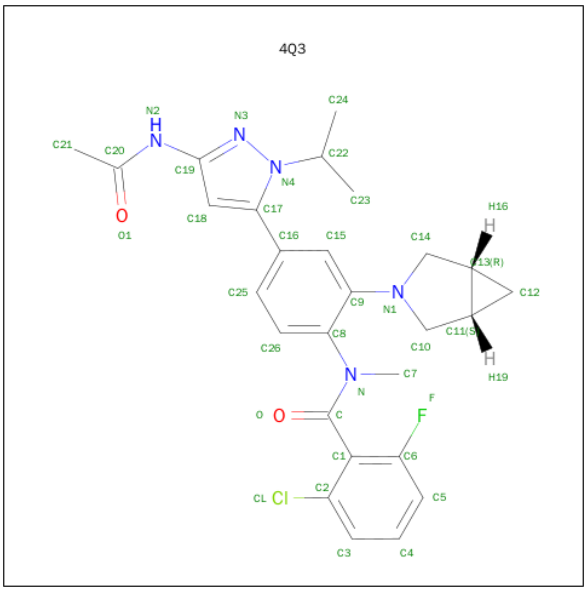
- Molecule 1 is a protein called Nuclear receptor ROR-gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	1	0
			1820	1150	328	328	14			
1	B	222	Total	C	N	O	S	0	0	0
			1786	1132	320	320	14			
1	C	219	Total	C	N	O	S	0	0	0
			1745	1111	308	312	14			
1	D	215	Total	C	N	O	S	0	0	0
			1712	1086	303	309	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	263	GLY	-	expression tag	UNP P51449
A	264	SER	-	expression tag	UNP P51449
B	263	GLY	-	expression tag	UNP P51449
B	264	SER	-	expression tag	UNP P51449
C	263	GLY	-	expression tag	UNP P51449
C	264	SER	-	expression tag	UNP P51449
D	263	GLY	-	expression tag	UNP P51449
D	264	SER	-	expression tag	UNP P51449

- Molecule 2 is N-{4-[3-(acetylamino)-1-(propan-2-yl)-1H-pyrazol-5-yl]-2-[(1R,5S)-3-azabicyclo[3.1.0]hex-3-yl]phenyl}-2-chloro-6-fluoro-N-methylbenzamide (three-letter code: 4Q3) (formula: $C_{27}H_{29}ClFN_5O_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			36	27	1	1	5	2		
2	B	1	Total	C	Cl	F	N	O	0	0
			36	27	1	1	5	2		
2	C	1	Total	C	Cl	F	N	O	0	0
			36	27	1	1	5	2		
2	D	1	Total	C	Cl	F	N	O	0	0
			36	27	1	1	5	2		

- Molecule 3 is water.

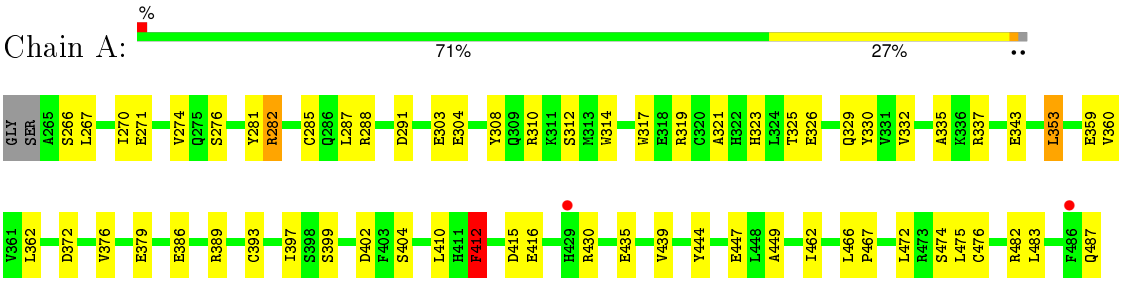
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	37	Total	O	0	0
			37	37		

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.

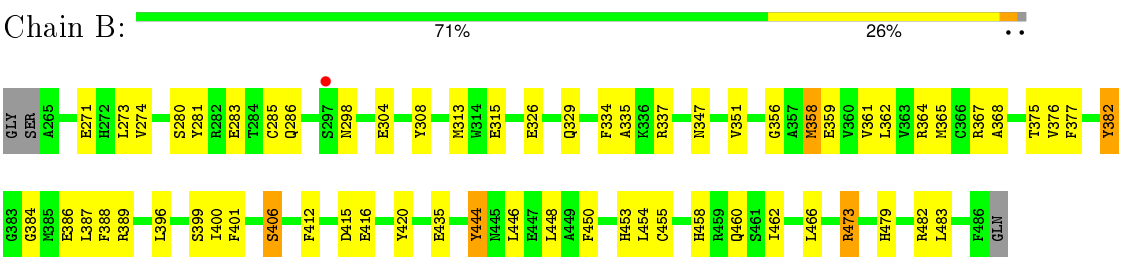
- Molecule 1: Nuclear receptor ROR-gamma

Chain A:



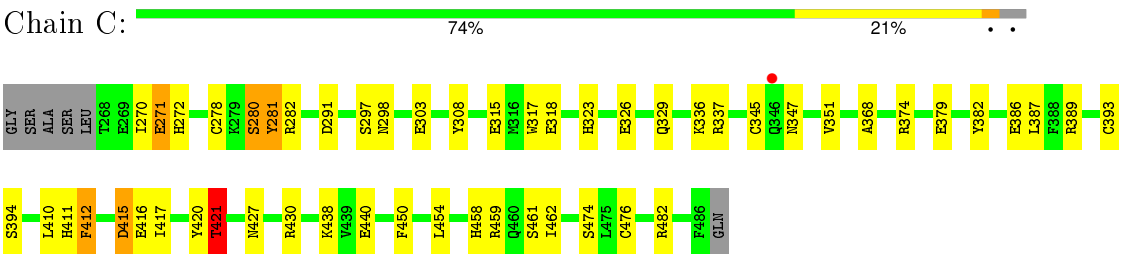
- Molecule 1: Nuclear receptor ROR-gamma

Chain B:



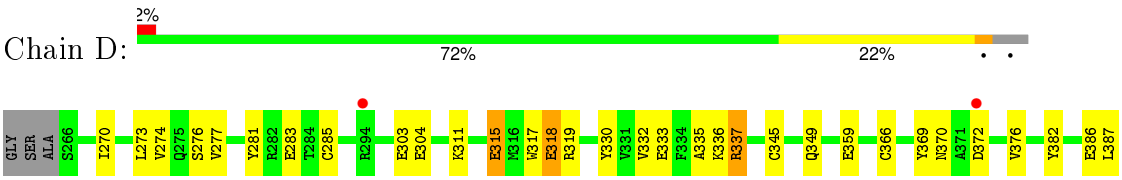
- Molecule 1: Nuclear receptor ROR-gamma

Chain C:



- Molecule 1: Nuclear receptor ROR-gamma

Chain D:




F388
S394
I397
S398
F401
D402
H405
F412
D415
E416
E435
E440
Y444
L448
L454
R459
Q460
S461
I462
K469
G470
S474
S477
V480
GLU
ARG
LEU
GLN
ILE
PHE
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	99.42Å 99.42Å 129.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.79 – 2.27 19.79 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.79-2.27) 99.9 (19.79-2.27)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.28Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.240 0.199 , 0.233	Depositor DCC
R_{free} test set	3397 reflections (5.43%)	DCC
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 33.4	EDS
Estimated twinning fraction	0.536 for H, K, L 0.464 for -H, -K, L 0.339 for -h,-k,l 0.117 for h,-h-k,-l 0.105 for -k,-h,-l	Xtriage
Reported twinning fraction	0.536 for H, K, L 0.464 for -H, -K, L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 65951 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7255	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: 4Q3

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	1.78	28/1856 (1.5%)	1.30	11/2496 (0.4%)
1	B	1.80	33/1821 (1.8%)	1.26	4/2454 (0.2%)
1	C	1.86	34/1780 (1.9%)	1.23	8/2400 (0.3%)
1	D	1.85	30/1746 (1.7%)	1.26	10/2352 (0.4%)
All	All	1.82	125/7203 (1.7%)	1.26	33/9702 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	416	GLU	CD-OE1	9.79	1.36	1.25
1	C	315	GLU	CD-OE2	9.44	1.36	1.25
1	A	276	SER	CA-CB	-8.85	1.39	1.52
1	D	276	SER	CA-CB	-8.77	1.39	1.52
1	C	416	GLU	CD-OE1	8.66	1.35	1.25
1	A	435	GLU	CD-OE1	8.63	1.35	1.25
1	C	386	GLU	CD-OE1	8.42	1.34	1.25
1	D	416	GLU	CD-OE1	8.24	1.34	1.25
1	C	281	TYR	CB-CG	-8.17	1.39	1.51
1	D	304	GLU	CD-OE2	8.08	1.34	1.25
1	D	415	ASP	CB-CG	8.08	1.68	1.51
1	C	450	PHE	CG-CD1	-7.89	1.26	1.38
1	B	304	GLU	CD-OE2	7.88	1.34	1.25
1	A	308	TYR	CE2-CZ	-7.74	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	TRP	N-CA	-7.58	1.31	1.46
1	B	415	ASP	CB-CG	7.48	1.67	1.51
1	A	335	ALA	C-O	7.32	1.37	1.23
1	D	440	GLU	CG-CD	7.26	1.62	1.51
1	A	337	ARG	CZ-NH1	7.26	1.42	1.33
1	B	356	GLY	C-O	7.19	1.35	1.23
1	B	335	ALA	C-O	7.03	1.36	1.23
1	C	461	SER	N-CA	-7.01	1.32	1.46
1	B	450	PHE	CG-CD1	-6.99	1.28	1.38
1	D	412	PHE	N-CA	-6.74	1.32	1.46
1	D	281	TYR	CB-CG	-6.71	1.41	1.51
1	C	271	GLU	CD-OE1	6.53	1.32	1.25
1	C	440	GLU	CA-C	-6.51	1.36	1.52
1	B	271	GLU	CD-OE2	6.51	1.32	1.25
1	A	281	TYR	CB-CG	-6.47	1.42	1.51
1	B	399	SER	N-CA	6.39	1.59	1.46
1	A	386	GLU	CD-OE2	6.36	1.32	1.25
1	C	389	ARG	CZ-NH2	6.34	1.41	1.33
1	A	444	TYR	CZ-OH	6.29	1.48	1.37
1	A	304	GLU	CD-OE2	6.28	1.32	1.25
1	D	461	SER	CB-OG	6.22	1.50	1.42
1	C	329	GLN	N-CA	-6.22	1.33	1.46
1	C	416	GLU	CD-OE2	6.20	1.32	1.25
1	D	336	LYS	C-O	-6.17	1.11	1.23
1	A	330	TYR	CE1-CZ	6.13	1.46	1.38
1	B	386	GLU	CD-OE2	6.08	1.32	1.25
1	B	416	GLU	CD-OE2	6.06	1.32	1.25
1	A	444	TYR	CB-CG	6.05	1.60	1.51
1	B	283	GLU	CD-OE2	6.04	1.32	1.25
1	D	435	GLU	CD-OE1	6.03	1.32	1.25
1	B	368	ALA	CA-CB	6.03	1.65	1.52
1	A	271	GLU	CG-CD	5.99	1.60	1.51
1	C	308	TYR	CE2-CZ	-5.99	1.30	1.38
1	D	281	TYR	CE2-CZ	-5.99	1.30	1.38
1	B	283	GLU	CD-OE1	5.97	1.32	1.25
1	B	435	GLU	CD-OE1	5.97	1.32	1.25
1	C	272	HIS	N-CA	-5.97	1.34	1.46
1	D	315	GLU	CG-CD	5.96	1.60	1.51
1	B	281	TYR	CB-CG	-5.95	1.42	1.51
1	D	382	TYR	CE1-CZ	5.95	1.46	1.38
1	B	313	MET	C-O	5.94	1.34	1.23
1	A	343	GLU	CG-CD	5.93	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	SER	CB-OG	5.92	1.50	1.42
1	B	382	TYR	CB-CG	5.92	1.60	1.51
1	A	447	GLU	CD-OE2	-5.90	1.19	1.25
1	D	386	GLU	CD-OE1	5.90	1.32	1.25
1	C	421	THR	N-CA	-5.85	1.34	1.46
1	C	326	GLU	CD-OE1	5.83	1.32	1.25
1	C	421	THR	CB-CG2	-5.81	1.33	1.52
1	D	274	VAL	C-O	5.81	1.34	1.23
1	C	336	LYS	C-O	-5.80	1.12	1.23
1	D	332	VAL	CA-CB	-5.71	1.42	1.54
1	A	353	LEU	N-CA	5.61	1.57	1.46
1	A	372	ASP	CB-CG	5.61	1.63	1.51
1	C	415	ASP	CB-CG	5.56	1.63	1.51
1	B	315	GLU	CD-OE2	5.55	1.31	1.25
1	C	368	ALA	CA-CB	5.53	1.64	1.52
1	B	337	ARG	CZ-NH1	5.51	1.40	1.33
1	D	317	TRP	N-CA	-5.50	1.35	1.46
1	C	318	GLU	CG-CD	5.50	1.60	1.51
1	B	444	TYR	CE1-CZ	5.46	1.45	1.38
1	B	326	GLU	CD-OE2	5.46	1.31	1.25
1	B	435	GLU	CG-CD	5.46	1.60	1.51
1	C	420	TYR	CE1-CZ	-5.45	1.31	1.38
1	C	315	GLU	CD-OE1	5.44	1.31	1.25
1	D	359	GLU	CG-CD	5.43	1.60	1.51
1	C	337	ARG	CZ-NH1	5.41	1.40	1.33
1	D	277	VAL	N-CA	-5.41	1.35	1.46
1	A	326	GLU	CG-CD	5.39	1.60	1.51
1	B	280	SER	C-O	-5.38	1.13	1.23
1	C	458	HIS	N-CA	5.38	1.57	1.46
1	C	382	TYR	CB-CG	5.37	1.59	1.51
1	D	330	TYR	C-O	5.37	1.33	1.23
1	D	317	TRP	CG-CD1	5.36	1.44	1.36
1	D	477	SER	CB-OG	-5.34	1.35	1.42
1	A	399	SER	CA-C	5.33	1.66	1.52
1	D	319	ARG	N-CA	-5.32	1.35	1.46
1	A	312	SER	N-CA	-5.30	1.35	1.46
1	A	329	GLN	C-O	-5.29	1.13	1.23
1	B	308	TYR	CZ-OH	5.28	1.46	1.37
1	B	377	PHE	C-O	-5.28	1.13	1.23
1	D	376	VAL	C-O	-5.27	1.13	1.23
1	B	446	LEU	C-O	5.26	1.33	1.23
1	C	315	GLU	CG-CD	5.26	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	393	CYS	CB-SG	-5.25	1.73	1.81
1	B	375	THR	N-CA	-5.22	1.35	1.46
1	D	335	ALA	C-O	5.22	1.33	1.23
1	A	415	ASP	CB-CG	5.21	1.62	1.51
1	D	460	GLN	C-O	-5.21	1.13	1.23
1	A	360	VAL	CB-CG2	-5.20	1.42	1.52
1	D	337	ARG	CZ-NH2	5.18	1.39	1.33
1	C	303	GLU	CD-OE1	5.17	1.31	1.25
1	C	326	GLU	CG-CD	5.15	1.59	1.51
1	A	416	GLU	CD-OE1	5.15	1.31	1.25
1	A	274	VAL	C-O	5.14	1.33	1.23
1	C	317	TRP	CZ3-CH2	5.14	1.48	1.40
1	B	389	ARG	CZ-NH2	5.13	1.39	1.33
1	A	412	PHE	N-CA	-5.13	1.36	1.46
1	C	281	TYR	CZ-OH	5.11	1.46	1.37
1	B	388	PHE	CG-CD1	-5.10	1.31	1.38
1	D	333	GLU	CD-OE1	5.10	1.31	1.25
1	A	474	SER	CB-OG	5.10	1.48	1.42
1	C	303	GLU	CD-OE2	5.07	1.31	1.25
1	B	334	PHE	CG-CD1	5.05	1.46	1.38
1	C	297	SER	CB-OG	5.04	1.48	1.42
1	D	460	GLN	CA-CB	5.03	1.65	1.53
1	B	359	GLU	CG-CD	5.02	1.59	1.51
1	B	384	GLY	N-CA	-5.02	1.38	1.46
1	D	318	GLU	CG-CD	5.02	1.59	1.51
1	C	280	SER	CA-CB	-5.01	1.45	1.52
1	B	406	SER	CB-OG	5.01	1.48	1.42

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	358	MET	CG-SD-CE	10.67	117.27	100.20
1	A	389	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	A	319	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	A	337	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	A	310	ARG	NE-CZ-NH2	-7.69	116.46	120.30
1	C	430	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	C	389	ARG	NE-CZ-NH1	-6.99	116.81	120.30
1	B	337	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	C	337	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	A	282	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	A	282	ARG	NE-CZ-NH1	6.81	123.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	476	CYS	CA-CB-SG	-6.01	103.19	114.00
1	D	337	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	C	459	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	402	ASP	CB-CG-OD1	5.79	123.51	118.30
1	D	416	GLU	OE1-CD-OE2	-5.64	116.53	123.30
1	D	285	CYS	CA-CB-SG	-5.59	103.93	114.00
1	B	455	CYS	CB-CA-C	-5.48	99.45	110.40
1	D	337	ARG	NE-CZ-NH1	-5.45	117.57	120.30
1	A	402	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	D	273	LEU	CB-CA-C	5.41	120.47	110.20
1	A	376	VAL	CG1-CB-CG2	-5.39	102.28	110.90
1	B	367	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	C	345	CYS	CA-CB-SG	5.35	123.63	114.00
1	D	459	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	439	VAL	CG1-CB-CG2	-5.32	102.39	110.90
1	D	444	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	C	412	PHE	CB-CA-C	-5.22	99.95	110.40
1	D	337	ARG	NH1-CZ-NH2	5.21	125.13	119.40
1	A	430	ARG	CD-NE-CZ	5.11	130.75	123.60
1	C	430	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	D	402	ASP	CB-CG-OD1	5.07	122.86	118.30
1	D	440	GLU	OE1-CD-OE2	-5.03	117.27	123.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	482	ARG	Peptide
1	A	483	LEU	Peptide

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	1820	0	1799	19	0
1	B	1786	0	1759	24	0
1	C	1745	0	1711	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1712	0	1681	11	0
2	A	36	0	29	0	0
2	B	36	0	29	3	0
2	C	36	0	29	2	0
2	D	36	0	29	5	0
3	A	11	0	0	0	0
3	B	37	0	0	3	0
All	All	7255	0	7066	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 5.

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:B:473:ARG:HG2	1:B:473:ARG:HH11	1.27	0.98
1:A:412:PHE:HZ	1:A:466:LEU:HD21	1.37	0.86
1:C:417:ILE:O	1:C:421:THR:HB	1.78	0.83
1:A:321:ALA:O	1:A:325:THR:HG23	1.84	0.77
1:A:412:PHE:CZ	1:A:466:LEU:HD21	2.26	0.70
2:D:501:4Q3:H15	2:D:501:4Q3:H26	1.73	0.70
1:B:473:ARG:NH1	1:B:473:ARG:HG2	1.95	0.69
1:B:285:CYS:O	1:B:286:GLN:HB3	1.92	0.68
1:A:362:LEU:HD21	1:A:475:LEU:HD23	1.76	0.67
1:D:369:TYR:OH	1:D:405:HIS:HD2	1.79	0.65
1:B:358:MET:HE3	1:B:361:VAL:HB	1.83	0.60
2:D:501:4Q3:H15	2:D:501:4Q3:C7	2.32	0.59
1:D:369:TYR:OH	1:D:405:HIS:CD2	2.58	0.57
1:C:347:ASN:O	1:C:351:VAL:HG23	2.06	0.56
1:C:454:LEU:HD21	1:C:462:ILE:HD11	1.88	0.55
1:A:410:LEU:HD23	1:A:412:PHE:CE1	2.41	0.55
1:B:473:ARG:CG	1:B:473:ARG:HH11	2.07	0.55
2:C:501:4Q3:H26	2:C:501:4Q3:H15	1.89	0.54
1:D:394:SER:O	1:D:398:SER:HB2	2.08	0.54
1:D:454:LEU:HD21	1:D:462:ILE:HD11	1.90	0.54
1:A:359:GLU:HB3	1:A:472:LEU:HD21	1.90	0.53
1:D:283:GLU:OE1	1:D:337:ARG:NH1	2.40	0.53
1:D:311:LYS:HD3	1:D:315:GLU:HG3	1.90	0.53
1:C:323:HIS:HE1	1:C:379:GLU:OE2	1.92	0.52
1:A:412:PHE:CE1	1:A:462:ILE:HD12	2.45	0.52
1:A:412:PHE:CZ	1:A:466:LEU:CD2	2.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:TYR:CZ	1:B:448:LEU:HD21	2.45	0.51
1:B:420:TYR:CE1	1:B:466:LEU:HD13	2.46	0.51
1:D:270:ILE:HG21	1:D:448:LEU:HD12	1.93	0.50
1:B:358:MET:O	1:B:362:LEU:HG	2.12	0.50
1:B:400:ILE:HG21	2:B:501:4Q3:H16	1.94	0.49
1:B:347:ASN:O	1:B:351:VAL:HG23	2.12	0.49
1:A:282:ARG:NH2	1:D:318:GLU:OE2	2.45	0.49
1:C:270:ILE:C	1:C:270:ILE:HD12	2.33	0.49
1:C:280:SER:O	1:C:281:TYR:C	2.50	0.49
1:B:396:LEU:HD21	1:B:479:HIS:HD2	1.77	0.48
1:A:393:CYS:O	1:A:397:ILE:HG12	2.12	0.48
1:B:376:VAL:O	1:B:382:TYR:HA	2.14	0.48
1:D:345:CYS:O	1:D:349:GLN:HG3	2.13	0.48
1:C:270:ILE:HD12	1:C:271:GLU:N	2.29	0.48
1:D:401:PHE:HE1	2:D:501:4Q3:H17	1.79	0.47
1:A:270:ILE:HD13	1:A:449:ALA:HA	1.95	0.47
1:B:387:LEU:HD23	1:B:387:LEU:O	2.13	0.47
1:A:266:SER:OG	1:A:267:LEU:N	2.47	0.47
1:B:473:ARG:NH2	3:B:601:HOH:O	2.29	0.46
1:A:412:PHE:HZ	1:A:466:LEU:CD2	2.16	0.46
1:B:364:ARG:NH1	3:B:604:HOH:O	2.46	0.46
1:B:387:LEU:C	1:B:387:LEU:HD23	2.35	0.46
1:A:323:HIS:HE1	1:A:379:GLU:OE2	1.99	0.46
1:B:454:LEU:HD21	1:B:462:ILE:HD11	1.97	0.45
1:B:365:MET:HE1	2:B:501:4Q3:C13	2.47	0.44
2:C:501:4Q3:H15	2:C:501:4Q3:C7	2.48	0.44
1:B:444:TYR:OH	1:B:448:LEU:HD21	2.18	0.44
1:B:401:PHE:HE1	2:B:501:4Q3:H17	1.84	0.43
1:D:388:PHE:HB2	1:D:397:ILE:HD13	2.01	0.43
1:A:285:CYS:O	1:A:287:LEU:N	2.49	0.43
2:D:501:4Q3:C14	2:D:501:4Q3:H26	2.46	0.42
1:B:479:HIS:CE1	1:B:483:LEU:HD11	2.54	0.42
1:A:332:VAL:HG22	1:A:353:LEU:HD22	2.01	0.42
1:A:266:SER:O	1:A:270:ILE:HG23	2.20	0.42
1:B:453:HIS:HE1	3:B:605:HOH:O	2.03	0.42
1:B:273:LEU:O	1:B:274:VAL:C	2.56	0.41
1:A:314:TRP:HH2	1:A:487:GLN:HB2	1.86	0.41
1:C:482:ARG:HD3	1:C:482:ARG:HA	1.74	0.41
1:C:410:LEU:O	1:C:411:HIS:C	2.59	0.41
1:A:288:ARG:NH2	1:A:291:ASP:OD2	2.54	0.41
1:B:458:HIS:HA	1:B:460:GLN:HE22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:501:4Q3:C14	2:D:501:4Q3:N	2.84	0.41
1:C:278:CYS:HB3	1:C:415:ASP:OD1	2.21	0.41

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	222/225 (99%)	215 (97%)	6 (3%)	1 (0%)	34 39
1	B	220/225 (98%)	213 (97%)	7 (3%)	0	100 100
1	C	217/225 (96%)	207 (95%)	10 (5%)	0	100 100
1	D	213/225 (95%)	204 (96%)	9 (4%)	0	100 100
All	All	872/900 (97%)	839 (96%)	32 (4%)	1 (0%)	56 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	467	PRO

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	197/200 (98%)	194 (98%)	3 (2%)	72 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	191/200 (96%)	185 (97%)	6 (3%)	47 62
1	C	185/200 (92%)	174 (94%)	11 (6%)	24 30
1	D	183/200 (92%)	176 (96%)	7 (4%)	40 53
All	All	756/800 (94%)	729 (96%)	27 (4%)	42 55

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	GLU
1	A	412	PHE
1	A	476	CYS
1	B	298	ASN
1	B	329	GLN
1	B	406	SER
1	B	412	PHE
1	B	473	ARG
1	B	482	ARG
1	C	282	ARG
1	C	291	ASP
1	C	298	ASN
1	C	374	ARG
1	C	387	LEU
1	C	394	SER
1	C	412	PHE
1	C	421	THR
1	C	427	ASN
1	C	438	LYS
1	C	474	SER
1	D	303	GLU
1	D	366	CYS
1	D	370	ASN
1	D	372	ASP
1	D	387	LEU
1	D	412	PHE
1	D	469	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	ASN

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Mol	Chain	Res	Type
1	A	323	HIS
1	A	370	ASN
1	A	405	HIS
1	A	452	HIS
1	A	484	GLN
1	B	405	HIS
1	B	441	GLN
1	B	445	ASN
1	B	453	HIS
1	B	460	GLN
1	B	479	HIS
1	C	298	ASN
1	C	323	HIS
1	C	405	HIS
1	C	427	ASN
1	D	370	ASN
1	D	405	HIS
1	D	434	GLN

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

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	4Q3	A	501	-	37,40,40	2.55	13 (35%)	51,60,60	2.41	17 (33%)
2	4Q3	B	501	-	37,40,40	2.58	14 (37%)	51,60,60	2.80	20 (39%)
2	4Q3	C	501	-	37,40,40	2.61	14 (37%)	51,60,60	2.51	19 (37%)
2	4Q3	D	501	-	37,40,40	2.46	13 (35%)	51,60,60	2.74	18 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4Q3	A	501	-	-	0/24/41/41	0/4/5/5
2	4Q3	B	501	-	-	0/24/41/41	0/4/5/5
2	4Q3	C	501	-	-	0/24/41/41	0/4/5/5
2	4Q3	D	501	-	-	0/24/41/41	0/4/5/5

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	4Q3	C8-N	-6.84	1.35	1.44
2	C	501	4Q3	C17-N4	-5.90	1.28	1.36
2	A	501	4Q3	C17-N4	-5.48	1.29	1.36
2	B	501	4Q3	C8-N	-5.28	1.37	1.44
2	B	501	4Q3	C17-N4	-5.26	1.29	1.36
2	D	501	4Q3	C18-C17	-5.08	1.30	1.39
2	D	501	4Q3	C17-N4	-4.32	1.31	1.36
2	C	501	4Q3	C9-N1	-3.91	1.32	1.41
2	A	501	4Q3	C15-C16	-3.58	1.33	1.39
2	A	501	4Q3	C18-C17	-3.48	1.33	1.39
2	D	501	4Q3	C9-N1	-3.27	1.33	1.41
2	B	501	4Q3	C-N	-3.15	1.30	1.36
2	D	501	4Q3	C8-N	-2.99	1.40	1.44
2	A	501	4Q3	C-N	-2.92	1.30	1.36
2	B	501	4Q3	C16-C17	-2.88	1.43	1.47
2	B	501	4Q3	C9-N1	-2.81	1.34	1.41
2	C	501	4Q3	C16-C17	-2.67	1.43	1.47
2	B	501	4Q3	C18-C17	-2.56	1.34	1.39
2	B	501	4Q3	C20-N2	-2.43	1.31	1.35
2	D	501	4Q3	C-N	-2.22	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	4Q3	C8-N	-2.22	1.41	1.44
2	A	501	4Q3	C9-N1	-2.15	1.36	1.41
2	C	501	4Q3	C-N	-2.14	1.32	1.36
2	C	501	4Q3	C18-C17	-2.09	1.35	1.39
2	D	501	4Q3	C1-C	2.30	1.54	1.51
2	A	501	4Q3	C14-N1	2.43	1.49	1.46
2	A	501	4Q3	C16-C17	2.51	1.52	1.47
2	A	501	4Q3	C8-C9	2.52	1.45	1.40
2	B	501	4Q3	C12-C13	2.76	1.57	1.49
2	D	501	4Q3	C21-C20	2.76	1.56	1.50
2	A	501	4Q3	C10-N1	2.78	1.50	1.46
2	C	501	4Q3	C1-C	2.78	1.55	1.51
2	B	501	4Q3	C26-C8	2.78	1.44	1.39
2	A	501	4Q3	C21-C20	2.89	1.56	1.50
2	B	501	4Q3	N3-N4	2.90	1.41	1.37
2	C	501	4Q3	C25-C16	2.95	1.45	1.39
2	D	501	4Q3	C1-C2	2.97	1.44	1.39
2	B	501	4Q3	O-C	3.07	1.28	1.22
2	C	501	4Q3	F-C6	3.42	1.44	1.35
2	D	501	4Q3	C10-N1	3.48	1.51	1.46
2	A	501	4Q3	C14-C13	3.61	1.58	1.53
2	D	501	4Q3	C8-C9	3.67	1.47	1.40
2	C	501	4Q3	C14-C13	3.84	1.58	1.53
2	D	501	4Q3	C14-C13	4.24	1.59	1.53
2	C	501	4Q3	C8-C9	4.63	1.48	1.40
2	C	501	4Q3	C1-C2	4.83	1.47	1.39
2	D	501	4Q3	N3-N4	4.89	1.43	1.37
2	B	501	4Q3	C14-N1	5.13	1.53	1.46
2	B	501	4Q3	C8-C9	5.17	1.49	1.40
2	C	501	4Q3	C14-N1	5.73	1.54	1.46
2	C	501	4Q3	C1-C6	5.84	1.47	1.39
2	B	501	4Q3	C1-C2	6.01	1.48	1.39
2	A	501	4Q3	C1-C6	6.72	1.48	1.39
2	D	501	4Q3	C1-C6	6.82	1.48	1.39

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	4Q3	C12-C13-C14	-8.90	102.91	115.50
2	C	501	4Q3	C19-N2-C20	-8.23	119.31	128.15
2	D	501	4Q3	C19-N3-N4	-7.57	99.11	104.13
2	A	501	4Q3	C24-C22-N4	-7.23	102.15	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	4Q3	C24-C22-N4	-6.88	102.59	111.46
2	C	501	4Q3	C15-C9-N1	-6.72	113.03	122.63
2	A	501	4Q3	C19-N3-N4	-6.53	99.80	104.13
2	B	501	4Q3	C19-N2-C20	-6.41	121.27	128.15
2	D	501	4Q3	C24-C22-N4	-6.31	103.32	111.46
2	C	501	4Q3	C12-C13-C14	-5.38	107.88	115.50
2	A	501	4Q3	C1-C2-CL	-5.34	111.99	119.66
2	B	501	4Q3	C15-C9-N1	-5.07	115.38	122.63
2	D	501	4Q3	C23-C22-N4	-4.95	105.08	111.46
2	D	501	4Q3	C25-C16-C17	-4.06	113.31	120.77
2	B	501	4Q3	C17-N4-N3	-4.06	109.02	111.84
2	D	501	4Q3	C15-C9-N1	-4.00	116.91	122.63
2	A	501	4Q3	O1-C20-C21	-3.92	114.86	122.07
2	B	501	4Q3	C26-C25-C16	-3.64	116.03	121.15
2	B	501	4Q3	C26-C8-N	-3.60	114.07	118.78
2	D	501	4Q3	C19-N2-C20	-3.59	124.29	128.15
2	D	501	4Q3	C13-C14-N1	-3.53	98.87	103.02
2	B	501	4Q3	C12-C13-C14	-3.40	110.68	115.50
2	B	501	4Q3	C13-C14-N1	-3.35	99.08	103.02
2	A	501	4Q3	C12-C13-C14	-3.27	110.88	115.50
2	B	501	4Q3	C25-C16-C17	-3.25	114.81	120.77
2	A	501	4Q3	C15-C9-N1	-3.05	118.27	122.63
2	D	501	4Q3	C1-C2-CL	-2.99	115.37	119.66
2	D	501	4Q3	C26-C8-N	-2.91	114.97	118.78
2	C	501	4Q3	C13-C14-N1	-2.87	99.65	103.02
2	D	501	4Q3	C7-N-C8	-2.76	112.67	116.68
2	C	501	4Q3	C26-C25-C16	-2.69	117.36	121.15
2	A	501	4Q3	C13-C14-N1	-2.56	100.02	103.02
2	B	501	4Q3	C16-C17-N4	-2.56	119.91	123.47
2	C	501	4Q3	C26-C8-N	-2.49	115.52	118.78
2	A	501	4Q3	C15-C9-C8	-2.47	116.69	120.25
2	C	501	4Q3	C2-C1-C6	-2.45	112.88	117.18
2	A	501	4Q3	C26-C25-C16	-2.34	117.86	121.15
2	C	501	4Q3	C1-C2-CL	-2.26	116.42	119.66
2	C	501	4Q3	C5-C6-C1	-2.23	119.29	123.36
2	D	501	4Q3	C2-C1-C6	-2.15	113.41	117.18
2	C	501	4Q3	C14-N1-C9	-2.05	119.67	122.82
2	D	501	4Q3	O1-C20-N2	2.08	125.63	123.08
2	C	501	4Q3	C14-N1-C10	2.16	115.13	112.21
2	A	501	4Q3	C21-C20-N2	2.17	118.14	115.01
2	D	501	4Q3	C12-C13-C11	2.31	62.70	59.43
2	A	501	4Q3	C16-C15-C9	2.37	123.99	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	4Q3	C4-C5-C6	2.65	123.01	118.43
2	A	501	4Q3	C3-C2-CL	2.68	124.00	118.40
2	D	501	4Q3	C7-N-C	2.75	124.41	118.53
2	B	501	4Q3	C7-N-C8	2.84	120.81	116.68
2	B	501	4Q3	C12-C11-C13	2.86	63.49	59.43
2	C	501	4Q3	C23-C22-C24	2.98	124.05	113.26
2	D	501	4Q3	C14-N1-C10	2.99	116.25	112.21
2	C	501	4Q3	C4-C5-C6	3.02	123.66	118.43
2	A	501	4Q3	C25-C16-C15	3.09	122.08	118.17
2	C	501	4Q3	F-C6-C1	3.09	123.12	118.13
2	C	501	4Q3	O-C-C1	3.10	125.15	119.17
2	B	501	4Q3	C8-C9-N1	3.11	124.06	120.45
2	A	501	4Q3	O1-C20-N2	3.18	126.97	123.08
2	B	501	4Q3	O-C-C1	3.29	125.52	119.17
2	C	501	4Q3	C25-C16-C15	3.38	122.46	118.17
2	A	501	4Q3	C7-N-C	3.45	125.89	118.53
2	C	501	4Q3	C3-C2-C1	3.50	126.50	121.79
2	A	501	4Q3	C8-C9-N1	3.53	124.55	120.45
2	D	501	4Q3	C25-C16-C15	3.66	122.81	118.17
2	A	501	4Q3	C17-N4-N3	3.67	114.39	111.84
2	B	501	4Q3	C17-N4-C22	3.80	134.31	126.24
2	C	501	4Q3	C8-C9-N1	3.86	124.93	120.45
2	D	501	4Q3	C9-C8-N	3.90	126.71	122.32
2	B	501	4Q3	C14-N1-C10	3.95	117.55	112.21
2	B	501	4Q3	C18-C17-N4	4.05	110.42	107.58
2	C	501	4Q3	C9-C8-N	4.66	127.56	122.32
2	B	501	4Q3	C25-C16-C15	5.48	125.11	118.17
2	B	501	4Q3	C9-C8-N	6.44	129.56	122.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	4Q3	3	0
2	C	501	4Q3	2	0
2	D	501	4Q3	5	0

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	223/225 (99%)	-0.21	2 (0%)	85	89	19, 39, 65, 87	4 (1%)
1	B	222/225 (98%)	-0.24	1 (0%)	91	94	20, 39, 64, 70	3 (1%)
1	C	219/225 (97%)	-0.27	1 (0%)	91	94	21, 38, 61, 79	5 (2%)
1	D	215/225 (95%)	-0.26	5 (2%)	64	71	20, 38, 61, 81	5 (2%)
All	All	879/900 (97%)	-0.25	9 (1%)	84	87	19, 39, 64, 87	17 (1%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	486	PHE	4.9
1	D	480	VAL	2.9
1	B	297	SER	2.5
1	D	294	ARG	2.4
1	D	372	ASP	2.2
1	A	429	HIS	2.1
1	D	470	GLY	2.1
1	C	346	GLN	2.0
1	D	474	SER	2.0

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	4Q3	C	501	36/36	0.94	0.15	0.84	28,34,52,72	0
2	4Q3	B	501	36/36	0.96	0.12	0.08	28,35,48,73	0
2	4Q3	D	501	36/36	0.95	0.12	0.08	30,38,50,78	0
2	4Q3	A	501	36/36	0.94	0.12	-0.04	29,42,55,85	0

6.5 Other polymers

There are no such residues in this entry.