Full wwPDB X-ray Structure Validation Report (i)

Feb 24, 2025 – 06:06 PM EST

PDB ID	:	9DEP
Title	:	USP7 in complex with macrocycle MC09
Authors	:	Ultsch, M.; Tenorio, C.A.; Dueber, E.C.; Harris, S.F.
Deposited on	:	2024-08-29
Resolution	:	2.57 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 (i)) were used in the production of this report:

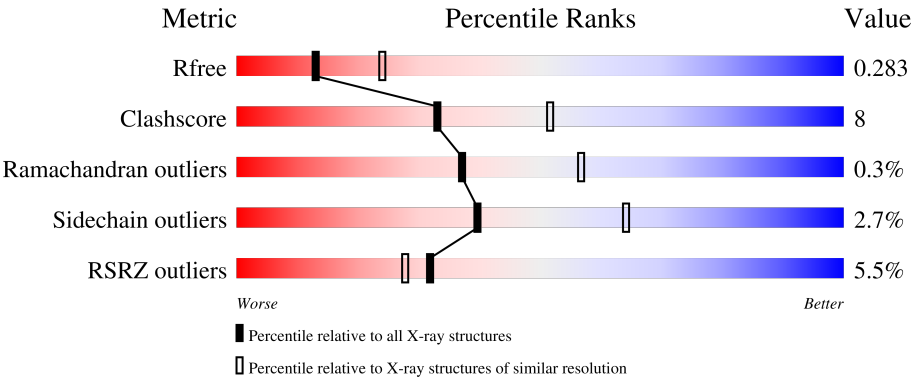
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.57 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.



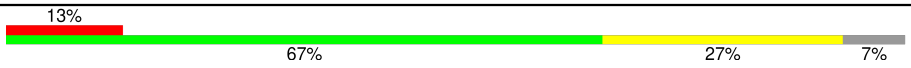
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (2.60-2.56)

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	368	2% 74% 15% • 9%
1	B	368	% 77% 16% 8%
1	E	368	12% 67% 20% • 12%
2	C	15	7% 93% 7%
2	D	15	87% 7% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	15	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8006 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 Ubiquitin carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2582	1634	429	503	16			
1	B	340	Total	C	N	O	S	0	0	0
			2675	1689	454	516	16			
1	E	323	Total	C	N	O	S	0	0	0
			2380	1507	390	468	15			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	MET	-	initiating methionine	UNP Q93009
A	188	GLY	-	expression tag	UNP Q93009
A	189	SER	-	expression tag	UNP Q93009
A	190	SER	-	expression tag	UNP Q93009
A	191	HIS	-	expression tag	UNP Q93009
A	192	HIS	-	expression tag	UNP Q93009
A	193	HIS	-	expression tag	UNP Q93009
A	194	HIS	-	expression tag	UNP Q93009
A	195	HIS	-	expression tag	UNP Q93009
A	196	HIS	-	expression tag	UNP Q93009
A	197	SER	-	expression tag	UNP Q93009
A	198	SER	-	expression tag	UNP Q93009
A	199	GLY	-	expression tag	UNP Q93009
A	200	LEU	-	expression tag	UNP Q93009
A	201	VAL	-	expression tag	UNP Q93009
A	202	PRO	-	expression tag	UNP Q93009
A	203	ARG	-	expression tag	UNP Q93009
A	204	GLY	-	expression tag	UNP Q93009
A	205	SER	-	expression tag	UNP Q93009
A	206	HIS	-	expression tag	UNP Q93009
A	207	MET	-	expression tag	UNP Q93009
B	187	MET	-	initiating methionine	UNP Q93009
B	188	GLY	-	expression tag	UNP Q93009

Continued on next page...

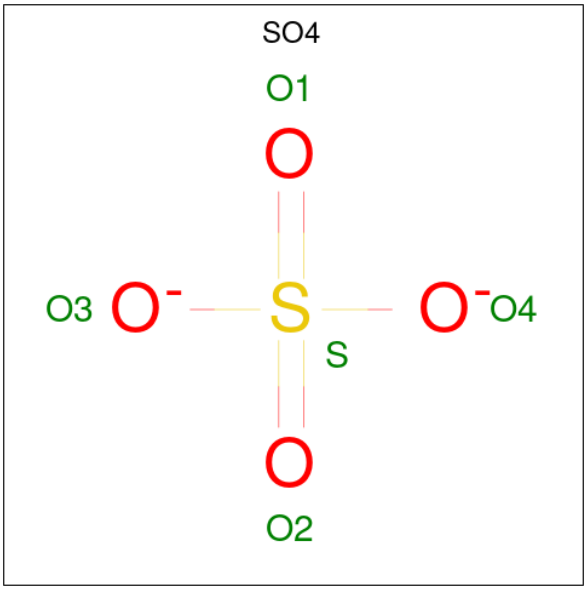
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	189	SER	-	expression tag	UNP Q93009
B	190	SER	-	expression tag	UNP Q93009
B	191	HIS	-	expression tag	UNP Q93009
B	192	HIS	-	expression tag	UNP Q93009
B	193	HIS	-	expression tag	UNP Q93009
B	194	HIS	-	expression tag	UNP Q93009
B	195	HIS	-	expression tag	UNP Q93009
B	196	HIS	-	expression tag	UNP Q93009
B	197	SER	-	expression tag	UNP Q93009
B	198	SER	-	expression tag	UNP Q93009
B	199	GLY	-	expression tag	UNP Q93009
B	200	LEU	-	expression tag	UNP Q93009
B	201	VAL	-	expression tag	UNP Q93009
B	202	PRO	-	expression tag	UNP Q93009
B	203	ARG	-	expression tag	UNP Q93009
B	204	GLY	-	expression tag	UNP Q93009
B	205	SER	-	expression tag	UNP Q93009
B	206	HIS	-	expression tag	UNP Q93009
B	207	MET	-	expression tag	UNP Q93009
E	187	MET	-	initiating methionine	UNP Q93009
E	188	GLY	-	expression tag	UNP Q93009
E	189	SER	-	expression tag	UNP Q93009
E	190	SER	-	expression tag	UNP Q93009
E	191	HIS	-	expression tag	UNP Q93009
E	192	HIS	-	expression tag	UNP Q93009
E	193	HIS	-	expression tag	UNP Q93009
E	194	HIS	-	expression tag	UNP Q93009
E	195	HIS	-	expression tag	UNP Q93009
E	196	HIS	-	expression tag	UNP Q93009
E	197	SER	-	expression tag	UNP Q93009
E	198	SER	-	expression tag	UNP Q93009
E	199	GLY	-	expression tag	UNP Q93009
E	200	LEU	-	expression tag	UNP Q93009
E	201	VAL	-	expression tag	UNP Q93009
E	202	PRO	-	expression tag	UNP Q93009
E	203	ARG	-	expression tag	UNP Q93009
E	204	GLY	-	expression tag	UNP Q93009
E	205	SER	-	expression tag	UNP Q93009
E	206	HIS	-	expression tag	UNP Q93009
E	207	MET	-	expression tag	UNP Q93009

- Molecule 2 is a protein called Macrocycle peptide MC09.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	S	0	0	0
			121	81	21	18	1			
2	D	14	Total	C	N	O	S	0	0	0
			122	81	23	17	1			
2	F	14	Total	C	N	O	S	0	0	0
			104	66	20	17	1			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	O	S		0	0
			5	4	1			

- Molecule 4 is water.

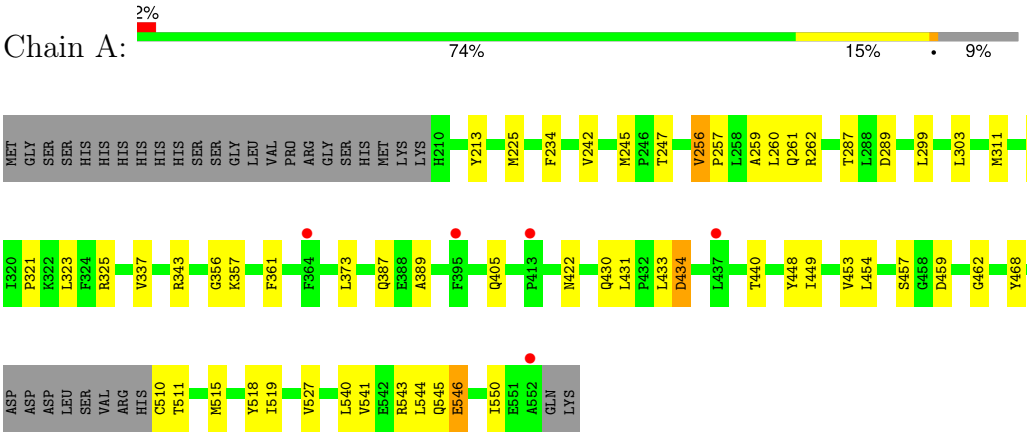
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	8	Total	O	0	0
			8	8		
4	C	1	Total	O	0	0
			1	1		
4	E	3	Total	O	0	0
			3	3		

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.

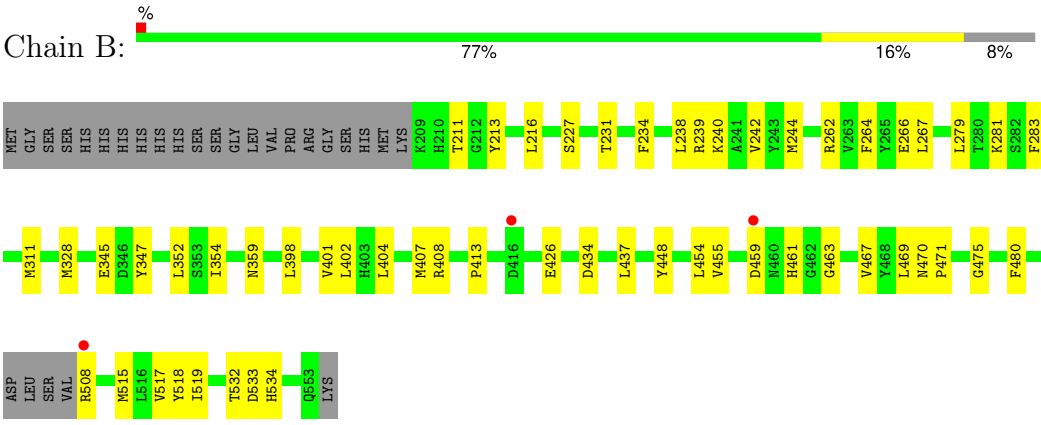
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7

Chain A:



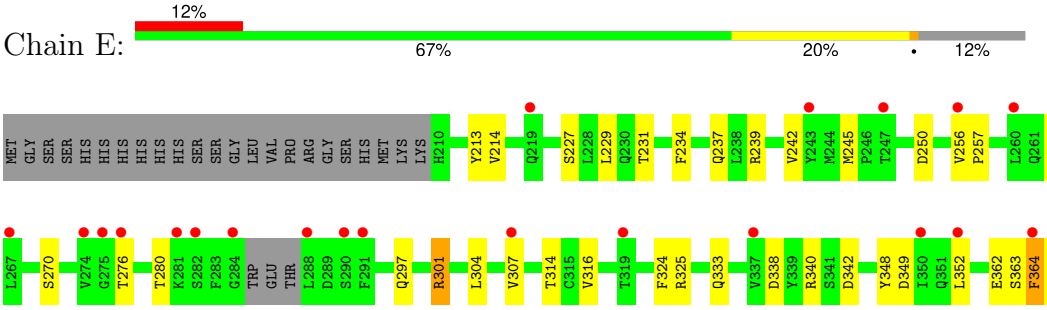
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7

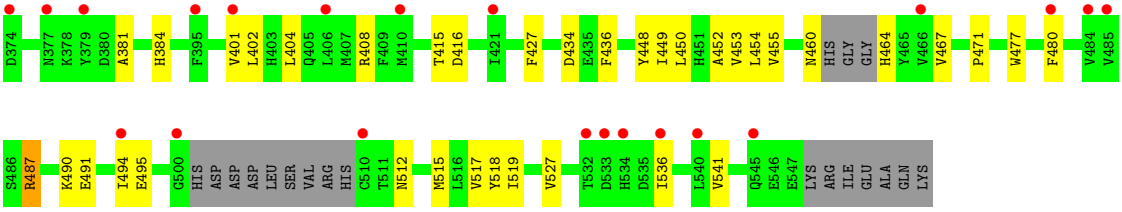
Chain B:



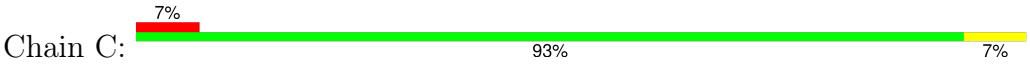
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7

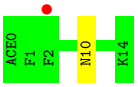
Chain E:



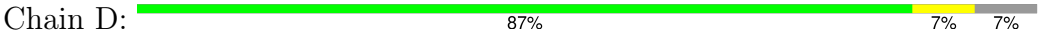


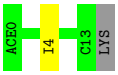
• Molecule 2: Macrocycle peptide MC09



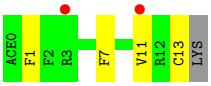


• Molecule 2: Macrocycle peptide MC09





• Molecule 2: Macrocycle peptide MC09



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	245.00Å 68.85Å 76.05Å 90.00° 105.21° 90.00°	Depositor
Resolution (Å)	73.39 – 2.57 73.39 – 2.57	Depositor EDS
% Data completeness (in resolution range)	69.2 (73.39-2.57) 69.2 (73.39-2.57)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.247 , 0.284 0.249 , 0.283	Depositor DCC
R_{free} test set	1936 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	68.2	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 55.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.005 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8006	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.72% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, SO4

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	0/2638	0.48	0/3589
1	B	0.26	0/2733	0.49	0/3707
1	E	0.26	0/2429	0.48	0/3320
2	C	0.28	0/122	0.56	0/164
2	D	0.28	0/123	0.63	0/164
2	F	0.27	0/103	0.62	0/139
All	All	0.26	0/8148	0.49	0/11083

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	2582	0	2378	38	0
1	B	2675	0	2504	33	0
1	E	2380	0	2063	47	0
2	C	121	0	111	0	0
2	D	122	0	120	2	0
2	F	104	0	95	1	0
3	B	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	5	0	0	0	0
4	B	8	0	0	0	0
4	C	1	0	0	0	0
4	E	3	0	0	3	0
All	All	8006	0	7271	117	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 8.

All (117) 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:E:452:ALA:HB3	1:E:517:VAL:HB	1.71	0.71
1:E:450:LEU:HD22	1:E:477:TRP:HH2	1.57	0.69
1:B:413:PRO:HD3	2:D:4:ILE:HD12	1.78	0.66
1:A:457:SER:HB2	1:A:511:THR:HG23	1.76	0.66
1:A:337:VAL:HG22	1:A:387:GLN:HG2	1.79	0.64
1:E:450:LEU:HD21	1:E:453:VAL:HG23	1.79	0.64
1:E:494:ILE:HB	4:E:601:HOH:O	2.02	0.60
1:A:247:THR:HG21	1:A:261:GLN:OE1	2.02	0.59
1:E:467:VAL:HG13	1:E:480:PHE:HB2	1.84	0.59
1:A:259:ALA:HA	1:A:262:ARG:HH12	1.67	0.58
1:B:459:ASP:HB2	1:B:463:GLY:H	1.69	0.58
1:E:237:GLN:HB2	1:E:527:VAL:HA	1.84	0.58
1:A:448:TYR:HB3	1:A:518:TYR:HB3	1.85	0.57
1:E:454:LEU:HB2	1:E:515:MET:HB3	1.86	0.57
1:A:343:ARG:NH1	1:E:495:GLU:HG2	2.19	0.56
1:E:415:THR:HG22	1:E:416:ASP:H	1.71	0.56
1:E:477:TRP:N	1:E:487:ARG:HH21	2.04	0.55
1:E:229:LEU:HD23	1:E:263:VAL:HG11	1.87	0.55
1:E:490:LYS:HD3	4:E:601:HOH:O	2.06	0.54
1:E:262:ARG:O	1:E:266:GLU:HG2	2.08	0.54
1:E:491:GLU:HA	4:E:601:HOH:O	2.06	0.54
1:A:259:ALA:HA	1:A:262:ARG:NH1	2.24	0.53
1:E:448:TYR:HB3	1:E:518:TYR:HB3	1.91	0.53
1:E:519:ILE:HG21	1:E:527:VAL:HG11	1.91	0.53
1:B:454:LEU:HB2	1:B:515:MET:HB3	1.91	0.53
1:E:245:MET:SD	1:E:307:VAL:HG23	2.49	0.52
1:A:319:THR:O	1:A:323:LEU:HD12	2.10	0.52
1:B:234:PHE:HD2	1:B:469:LEU:HD13	1.75	0.52
1:A:422:ASN:ND2	1:A:510:CYS:HB3	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:LEU:HG	1:B:404:LEU:HD21	1.91	0.51
1:E:427:PHE:CE1	1:E:494:ILE:HG23	2.45	0.51
1:B:467:VAL:HG13	1:B:480:PHE:HB2	1.91	0.51
1:A:356:GLY:C	1:A:357:LYS:HE2	2.31	0.51
1:B:242:VAL:HG11	1:B:264:PHE:HD2	1.76	0.51
1:A:319:THR:HG22	1:A:323:LEU:HD11	1.94	0.50
1:E:314:THR:HG23	1:E:316:VAL:H	1.75	0.50
1:B:242:VAL:HG11	1:B:264:PHE:CD2	2.47	0.50
1:A:540:LEU:O	1:A:544:LEU:HG	2.12	0.50
1:A:287:THR:HG22	1:A:289:ASP:H	1.77	0.50
1:E:352:LEU:HB3	1:E:363:SER:OG	2.12	0.50
1:B:532:THR:HG23	1:B:534:HIS:H	1.76	0.50
1:A:321:PRO:O	1:A:325:ARG:HB3	2.13	0.49
1:E:297:GLN:O	1:E:301:ARG:HD3	2.12	0.49
1:E:408:ARG:HD3	1:E:512:ASN:ND2	2.27	0.49
1:E:364:PHE:HB3	1:E:436:PHE:CE2	2.47	0.49
1:E:333:GLN:HB2	1:E:340:ARG:NH1	2.28	0.49
1:A:462:GLY:HA3	1:B:508:ARG:NH2	2.28	0.48
1:B:448:TYR:HB3	1:B:518:TYR:HB3	1.95	0.48
1:E:234:PHE:CD1	1:E:471:PRO:HB3	2.47	0.48
1:A:373:LEU:HD12	1:A:389:ALA:HB3	1.96	0.48
1:B:262:ARG:O	1:B:266:GLU:HG2	2.14	0.48
1:B:413:PRO:CD	2:D:4:ILE:HD12	2.44	0.48
1:E:402:LEU:HG	1:E:404:LEU:HD13	1.95	0.48
1:E:325:ARG:HB2	1:E:348:TYR:HE1	1.79	0.47
1:E:231:THR:HG21	1:E:517:VAL:HG21	1.96	0.47
1:E:304:LEU:HA	1:E:307:VAL:HG12	1.97	0.47
1:B:470:ASN:HD22	1:B:475:GLY:H	1.62	0.47
1:E:401:VAL:HG22	1:E:519:ILE:HG12	1.97	0.47
1:B:216:LEU:HD21	1:B:267:LEU:HD21	1.96	0.47
1:A:453:VAL:HG13	1:A:468:TYR:HB2	1.96	0.47
1:B:359:ASN:HB3	1:B:426:GLU:HB2	1.96	0.47
1:A:314:THR:HG23	1:A:316:VAL:H	1.80	0.46
1:B:231:THR:HG21	1:B:517:VAL:HG21	1.97	0.46
1:B:279:LEU:HG	1:B:283:PHE:HE2	1.80	0.45
1:A:546:GLU:O	1:A:550:ILE:HD12	2.16	0.45
1:B:211:THR:HG22	1:B:487:ARG:HG2	1.99	0.45
1:B:213:TYR:CZ	1:B:471:PRO:HG2	2.52	0.45
1:B:238:LEU:O	1:B:242:VAL:HG12	2.17	0.45
1:B:459:ASP:HB3	1:B:461:HIS:H	1.82	0.45
1:E:229:LEU:CD2	1:E:263:VAL:HG11	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:408:ARG:NH1	1:E:512:ASN:HD22	2.15	0.45
1:A:405:GLN:HG3	1:A:515:MET:HG3	1.99	0.45
1:E:227:SER:HB3	1:E:467:VAL:HB	1.98	0.45
1:A:213:TYR:CZ	1:A:471:PRO:HG2	2.52	0.44
1:A:260:LEU:HD22	1:A:303:LEU:HD23	1.99	0.44
1:E:213:TYR:CZ	1:E:471:PRO:HG2	2.52	0.44
1:A:541:VAL:O	1:A:545:GLN:HG3	2.16	0.44
1:A:434:ASP:OD2	1:A:440:THR:HB	2.17	0.44
1:B:307:VAL:O	1:B:311:MET:HG3	2.17	0.44
1:A:213:TYR:CE2	1:A:471:PRO:HG2	2.53	0.44
1:B:328:MET:HE3	1:B:345:GLU:HG3	1.99	0.44
1:E:453:VAL:HG12	1:E:455:VAL:HG23	2.00	0.44
1:A:319:THR:HG22	1:A:323:LEU:CD1	2.47	0.43
1:A:454:LEU:HB2	1:A:515:MET:HB3	2.00	0.43
1:E:436:PHE:CD1	1:E:436:PHE:N	2.84	0.43
1:B:352:LEU:O	1:B:407:MET:HG2	2.18	0.43
1:A:256:VAL:HG22	1:A:257:PRO:HD3	1.99	0.43
1:A:430:GLN:HG3	1:A:449:ILE:HD13	2.01	0.43
1:B:347:TYR:OH	1:B:398:LEU:HD23	2.19	0.43
1:B:227:SER:HB3	1:B:467:VAL:HB	2.01	0.42
1:A:242:VAL:O	1:A:245:MET:HE2	2.19	0.42
1:A:431:LEU:HG	1:A:433:LEU:HG	2.00	0.42
1:A:225:MET:HG3	1:A:299:LEU:HD21	2.00	0.42
1:B:354:ILE:HD13	1:B:408:ARG:HG2	2.01	0.42
2:F:7:PHE:CG	2:F:11:VAL:HB	2.54	0.42
1:E:536:ILE:HD12	1:E:541:VAL:HG22	2.01	0.42
1:E:324:PHE:CD1	1:E:401:VAL:HB	2.55	0.42
1:A:311:MET:HG2	1:A:316:VAL:HG23	2.01	0.42
1:B:240:LYS:O	1:B:244:MET:HG2	2.20	0.42
1:B:401:VAL:HG22	1:B:519:ILE:HG12	2.02	0.42
1:E:450:LEU:HD22	1:E:477:TRP:CH2	2.47	0.42
1:B:239:ARG:HA	1:B:242:VAL:HG12	2.01	0.42
1:E:449:ILE:HD13	1:E:449:ILE:HA	1.86	0.42
1:A:453:VAL:CG1	1:A:468:TYR:HB2	2.50	0.41
1:E:362:GLU:O	1:E:365:VAL:HG12	2.20	0.41
1:E:242:VAL:O	1:E:245:MET:HE2	2.19	0.41
1:E:276:THR:O	1:E:280:THR:HG23	2.20	0.41
1:A:311:MET:O	1:A:314:THR:HG22	2.19	0.41
1:A:234:PHE:CE1	1:A:471:PRO:HB3	2.55	0.41
1:E:381:ALA:HB3	1:E:384:HIS:HB2	2.02	0.41
1:A:256:VAL:HA	1:A:259:ALA:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:256:VAL:HG13	1:E:257:PRO:HD3	2.02	0.41
1:B:292:MET:HE3	1:B:292:MET:HB3	1.84	0.41
1:B:437:LEU:HD23	1:B:437:LEU:HA	1.87	0.41
1:E:214:VAL:HG11	1:E:270:SER:O	2.20	0.41
1:A:519:ILE:HD13	1:A:527:VAL:HG11	2.02	0.40
1:E:415:THR:HG22	1:E:416:ASP:N	2.36	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	330/368 (90%)	310 (94%)	18 (6%)	2 (1%)	22 41
1	B	336/368 (91%)	324 (96%)	12 (4%)	0	100 100
1	E	315/368 (86%)	298 (95%)	17 (5%)	0	100 100
2	C	13/15 (87%)	12 (92%)	1 (8%)	0	100 100
2	D	12/15 (80%)	11 (92%)	1 (8%)	0	100 100
2	F	12/15 (80%)	10 (83%)	1 (8%)	1 (8%)	0 0
All	All	1018/1149 (89%)	965 (95%)	50 (5%)	3 (0%)	37 57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	1	PHE
1	A	546	GLU
1	A	471	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	270/332 (81%)	265 (98%)	5 (2%)	52 74
1	B	284/332 (86%)	280 (99%)	4 (1%)	62 81
1	E	229/332 (69%)	218 (95%)	11 (5%)	21 42
2	C	11/13 (85%)	10 (91%)	1 (9%)	7 15
2	D	12/13 (92%)	12 (100%)	0	100 100
2	F	9/13 (69%)	8 (89%)	1 (11%)	5 9
All	All	815/1035 (79%)	793 (97%)	22 (3%)	40 64

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	VAL
1	A	361	PHE
1	A	434	ASP
1	A	459	ASP
1	A	543	ARG
1	B	281	LYS
1	B	434	ASP
1	B	455	VAL
1	B	533	ASP
2	C	10	ASN
1	E	239	ARG
1	E	250	ASP
1	E	301	ARG
1	E	338	ASP
1	E	342	ASP
1	E	349	ASP
1	E	364	PHE
1	E	434	ASP
1	E	460	ASN
1	E	464	HIS
1	E	487	ARG
2	F	13	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	ASN
1	A	422	ASN
1	B	294	HIS
1	B	372	GLN
1	E	230	GLN
1	E	384	HIS
1	E	460	ASN
1	E	512	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
3	SO4	B	601	-	4,4,4	0.67	0	6,6,6	0.04	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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	334/368 (90%)	0.34	7 (2%) 63 59	41, 68, 101, 138	0
1	B	340/368 (92%)	0.14	3 (0%) 81 78	35, 58, 87, 142	0
1	E	323/368 (87%)	1.09	44 (13%) 8 7	67, 92, 137, 168	0
2	C	14/15 (93%)	0.78	1 (7%) 23 20	50, 64, 86, 112	0
2	D	13/15 (86%)	0.31	0 100 100	47, 59, 81, 89	0
2	F	13/15 (86%)	1.38	2 (15%) 6 5	90, 104, 133, 147	0
All	All	1037/1149 (90%)	0.53	57 (5%) 32 28	35, 73, 119, 168	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	364	PHE	4.4
1	E	219	GLN	4.2
1	E	256	VAL	4.1
1	A	395	PHE	4.0
1	E	288	LEU	4.0
1	E	290	SER	3.8
1	E	260	LEU	3.5
1	E	377	ASN	3.4
1	E	282	SER	3.4
2	C	2	PHE	3.3
1	E	350	ILE	3.3
1	E	540	LEU	3.2
1	E	480	PHE	3.0
1	B	508	ARG	3.0
1	E	243	TYR	3.0
1	E	275	GLY	3.0
1	E	500	GLY	2.9
1	B	416	ASP	2.9
1	E	494	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	11	VAL	2.8
1	E	379	TYR	2.6
1	E	421	ILE	2.6
1	E	406	LEU	2.6
1	E	395	PHE	2.5
1	E	410	MET	2.5
1	E	352	LEU	2.5
1	E	484	VAL	2.5
1	E	284	GLY	2.5
2	F	3	ARG	2.5
1	E	319	THR	2.4
1	E	307	VAL	2.4
1	E	281	LYS	2.3
1	E	401	VAL	2.3
1	E	369	ALA	2.3
1	E	266	GLU	2.3
1	E	485	VAL	2.3
1	E	247	THR	2.3
1	B	459	ASP	2.3
1	E	267	LEU	2.2
1	A	316	VAL	2.2
1	E	274	VAL	2.2
1	E	466	VAL	2.2
1	A	500	GLY	2.2
1	E	532	THR	2.2
1	E	545	GLN	2.2
1	A	552	ALA	2.2
1	E	534	HIS	2.2
1	E	374	ASP	2.1
1	E	276	THR	2.1
1	E	510	CYS	2.1
1	A	437	LEU	2.1
1	A	364	PHE	2.1
1	E	533	ASP	2.1
1	E	536	ILE	2.0
1	E	337	VAL	2.0
1	A	413	PRO	2.0
1	E	291	PHE	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)

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. 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	B-factors(Å^2)	Q<0.9
3	SO4	B	601	5/5	0.63	0.13	101,109,113,118	0

6.5 Other polymers (i)

There are no such residues in this entry.