Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 06:37 AM EDT

PDB ID	:	5ODS
Title	:	Structure of a phosphoprotein-protein complex
Authors	:	Mukherjee, M.; Bayliss, R.
Deposited on	:	2017-07-06
Resolution	:	3.09 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:

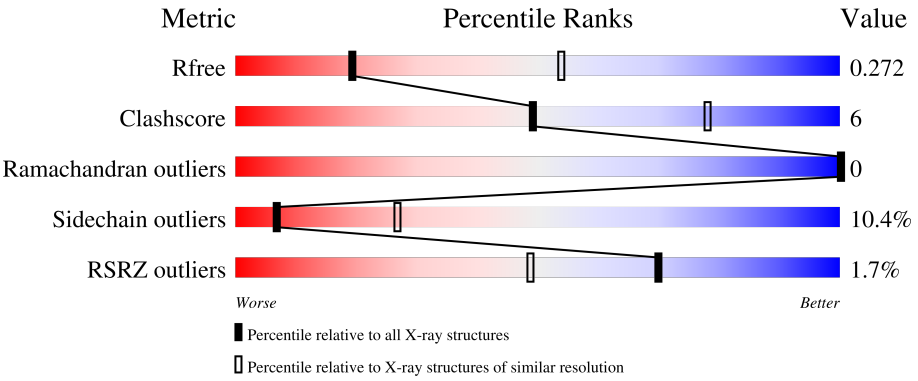
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.09 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	574	79% 19%
1	B	574	% 75% 21%
1	C	574	4% 78% 16%
1	D	574	2% 77% 20%
2	E	18	78% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	18	6% 78% 17% 6%
2	G	18	6% 78% 22%
2	H	18	6% 72% 17% 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18224 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 Clathrin heavy chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	0	0	0
			4474	2854	761	834	25			
1	B	567	Total	C	N	O	S	0	0	0
			4417	2823	748	821	25			
1	C	554	Total	C	N	O	S	0	0	0
			4321	2764	735	797	25			
1	D	571	Total	C	N	O	S	0	0	0
			4432	2831	751	825	25			

- Molecule 2 is a protein called LYS-GLU-SER-ALA-LEU-ARG-LYS-GLN-SEP-LEU-TYR-LEU-LYS-PHE-ASP-PRO-LEU-LEU.

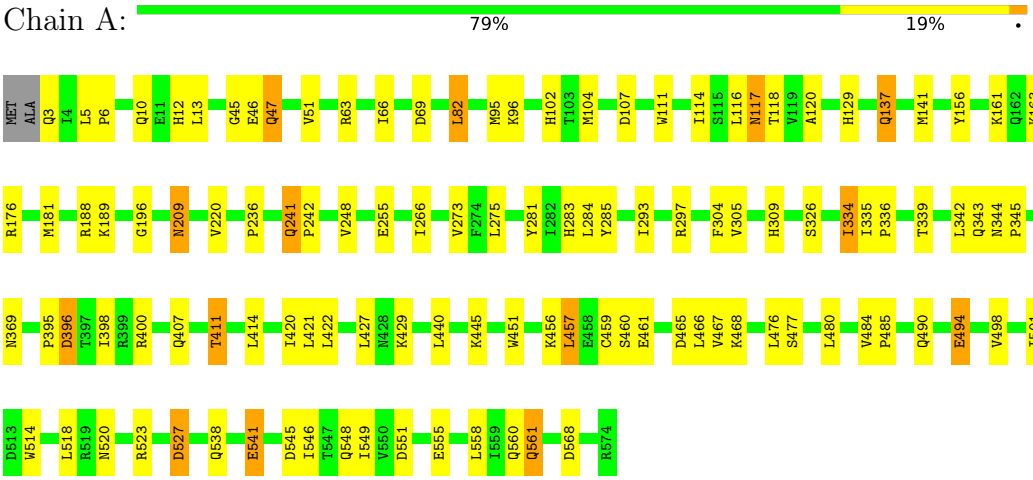
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			147	95	24	27	1			
2	F	18	Total	C	N	O	P	0	0	0
			143	92	23	27	1			
2	G	18	Total	C	N	O	P	0	0	0
			143	92	23	27	1			
2	H	18	Total	C	N	O	P	0	0	0
			147	95	24	27	1			

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.

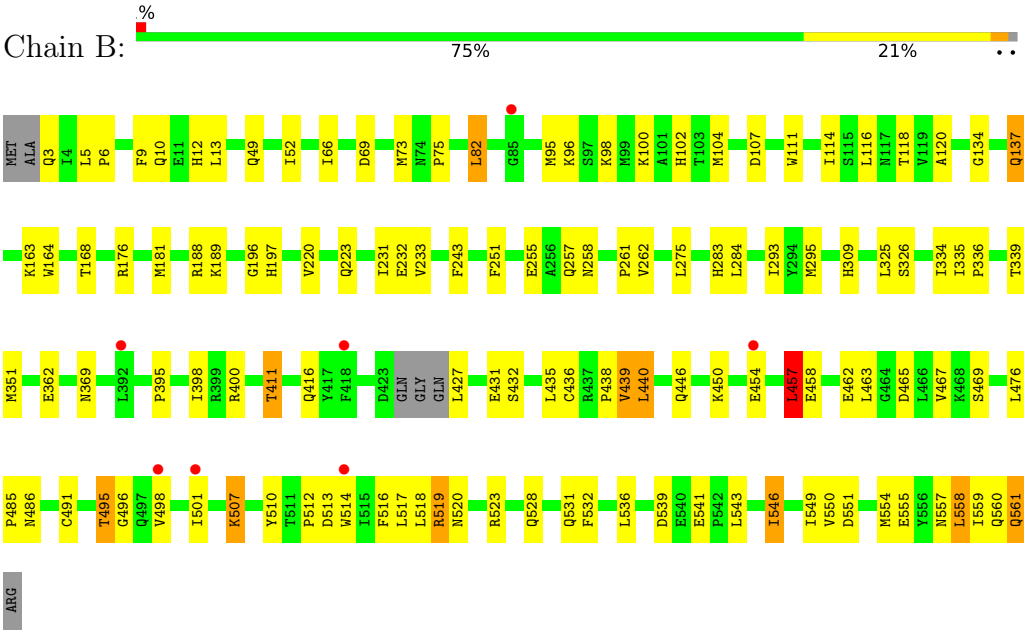
• Molecule 1: Clathrin heavy chain 1

Chain A:



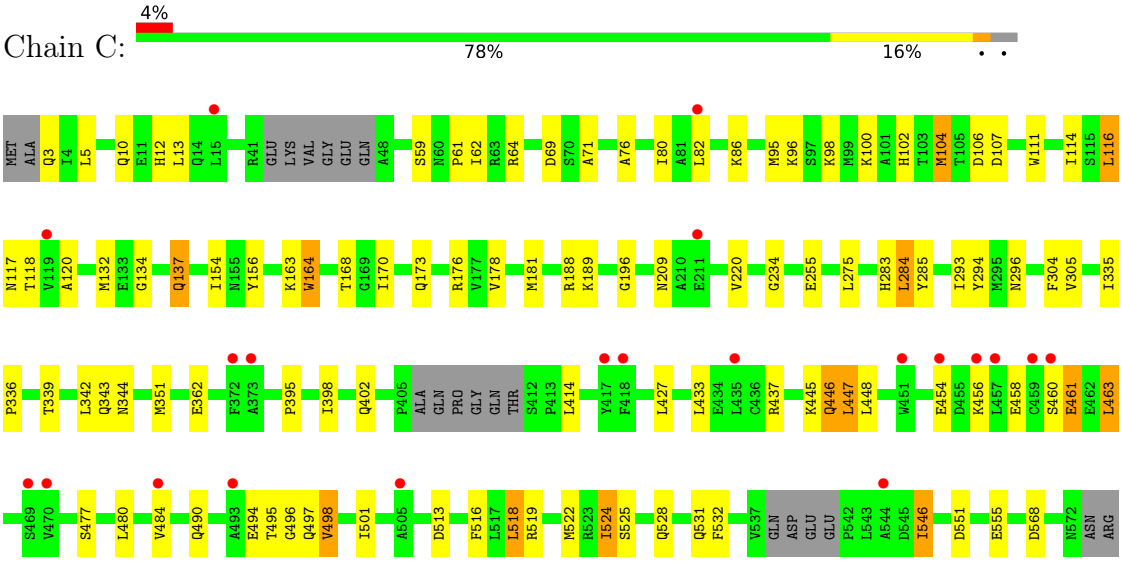
• Molecule 1: Clathrin heavy chain 1

Chain B:



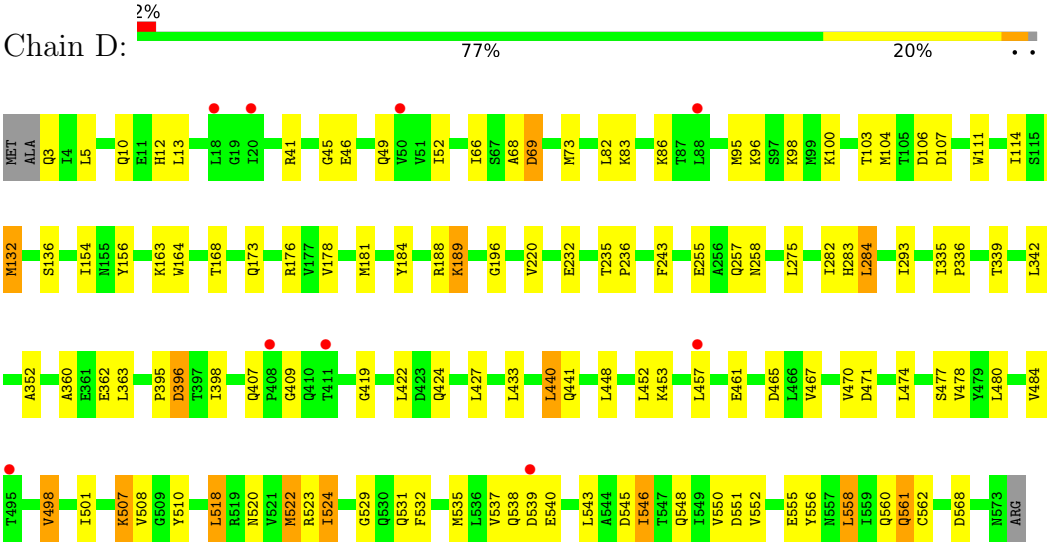
• Molecule 1: Clathrin heavy chain 1

Chain C:



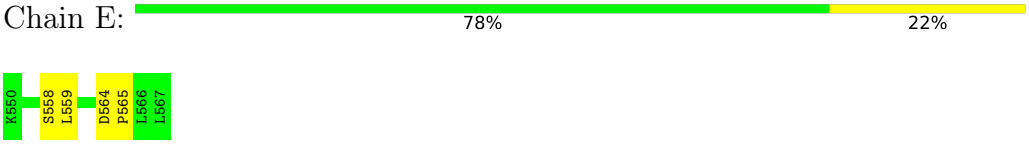
• Molecule 1: Clathrin heavy chain 1

Chain D:



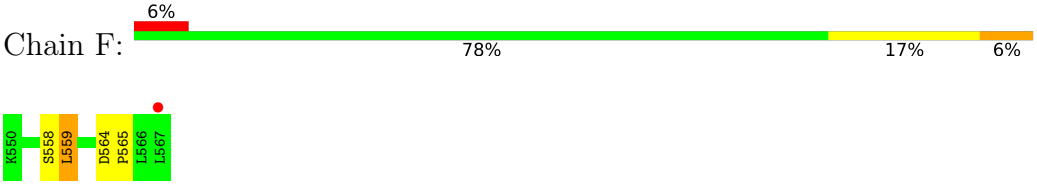
• Molecule 2: LYS-GLU-SER-ALA-LEU-ARG-LYS-GLN-SEP-LEU-TYR-LEU-LYS-PHE-ASP-PRO-LEU-LEU

Chain E:



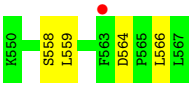
• Molecule 2: LYS-GLU-SER-ALA-LEU-ARG-LYS-GLN-SEP-LEU-TYR-LEU-LYS-PHE-ASP-PRO-LEU-LEU

Chain F:



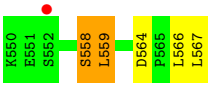
• Molecule 2: LYS-GLU-SER-ALA-LEU-ARG-LYS-GLN-SEP-LEU-TYR-LEU-LYS-PHE-ASP-PRO-LEU-LEU

Chain G:



• Molecule 2: LYS-GLU-SER-ALA-LEU-ARG-LYS-GLN-SEP-LEU-TYR-LEU-LYS-PHE-ASP-PRO-LEU-LEU

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	115.52Å 120.04Å 123.13Å 90.00° 95.72° 90.00°	Depositor
Resolution (Å)	61.26 – 3.09 61.26 – 3.09	Depositor EDS
% Data completeness (in resolution range)	98.7 (61.26-3.09) 98.7 (61.26-3.09)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.221 , 0.269 0.225 , 0.272	Depositor DCC
R_{free} test set	2888 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	99.4	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 84.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18224	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: SEP

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	0.29	0/4564	0.59	2/6194 (0.0%)
1	B	0.31	0/4506	0.59	2/6118 (0.0%)
1	C	0.29	0/4405	0.57	0/5974
1	D	0.32	0/4522	0.62	1/6143 (0.0%)
2	E	0.23	0/138	0.54	0/183
2	F	0.28	0/134	0.60	0/179
2	G	0.23	0/134	0.54	0/179
2	H	0.24	0/138	0.43	0/183
All	All	0.30	0/18541	0.59	5/25153 (0.0%)

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	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	241	GLN	C-N-CD	-7.09	105.01	120.60
1	B	457	LEU	CA-CB-CG	6.73	130.78	115.30
1	D	556	TYR	N-CA-C	6.11	127.49	111.00
1	B	440	LEU	CA-CB-CG	5.82	128.69	115.30
1	A	241	GLN	C-N-CA	5.31	144.29	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	GLN	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	4474	0	4479	50	0
1	B	4417	0	4411	60	0
1	C	4321	0	4336	47	0
1	D	4432	0	4414	60	0
2	E	147	0	148	1	0
2	F	143	0	137	2	0
2	G	143	0	137	1	0
2	H	147	0	148	4	0
All	All	18224	0	18210	216	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 6.

All (216) 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:C:460:SER:H	1:C:463:LEU:HD11	1.43	0.82
1:D:537:VAL:HG23	1:D:538:GLN:HG2	1.65	0.78
1:D:275:LEU:HB3	1:D:283:HIS:HB2	1.69	0.74
1:B:275:LEU:HB3	1:B:283:HIS:HB2	1.69	0.73
1:C:494:GLU:HA	1:C:524:ILE:HG21	1.70	0.73
1:D:558:LEU:HB3	1:D:561:GLN:HG3	1.71	0.73
1:A:275:LEU:HB3	1:A:283:HIS:HB2	1.70	0.71
1:C:275:LEU:HB3	1:C:283:HIS:HB2	1.72	0.71
1:D:539:ASP:OD1	1:D:540:GLU:N	2.24	0.70
1:C:402:GLN:HA	1:C:414:LEU:HD11	1.71	0.70
1:A:490:GLN:O	1:A:494:GLU:HG2	1.91	0.70
1:B:197:HIS:HB2	1:B:261:PRO:HG2	1.73	0.69
1:B:546:ILE:HD12	1:B:546:ILE:H	1.59	0.68
1:B:75:PRO:HG2	1:B:116:LEU:HD23	1.75	0.68
1:D:471:ASP:OD1	1:D:474:LEU:N	2.18	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:ILE:HD12	1:A:549:ILE:HD11	1.78	0.66
1:C:546:ILE:HD12	1:C:546:ILE:H	1.61	0.65
1:C:284:LEU:HB3	1:C:293:ILE:O	1.97	0.64
1:C:86:LYS:NZ	1:C:104:MET:O	2.27	0.64
1:A:527:ASP:OD1	1:A:527:ASP:N	2.31	0.64
1:D:41:ARG:NH2	1:D:68:ALA:O	2.31	0.64
1:D:522:MET:HE3	1:D:529:GLY:HA3	1.81	0.63
1:D:551:ASP:O	1:D:555:GLU:HG3	1.99	0.63
1:D:453:LYS:HD2	2:H:566:LEU:HD13	1.80	0.62
1:D:507:LYS:HE3	2:H:559:LEU:HG	1.82	0.62
1:C:519:ARG:NH1	1:C:555:GLU:OE1	2.32	0.61
1:D:284:LEU:HB3	1:D:293:ILE:O	2.00	0.61
1:B:432:SER:HB3	1:B:457:LEU:HD11	1.83	0.61
1:C:454:GLU:HB3	1:C:456:LYS:HG2	1.84	0.60
1:B:507:LYS:HG2	2:F:559:LEU:HD21	1.84	0.59
1:B:558:LEU:HD12	1:B:561:GLN:HE21	1.66	0.59
1:A:117:ASN:ND2	1:A:117:ASN:O	2.36	0.58
1:A:396:ASP:OD1	1:A:396:ASP:N	2.37	0.58
1:C:498:VAL:HA	1:C:501:ILE:HD12	1.85	0.58
1:C:463:LEU:HD13	1:C:463:LEU:H	1.68	0.58
1:B:395:PRO:HA	1:B:398:ILE:HD12	1.85	0.58
1:A:168:THR:HG23	1:A:181:MET:HG2	1.86	0.58
1:D:349:LEU:HG	1:D:363:LEU:HB3	1.86	0.57
1:A:558:LEU:HB3	1:A:561:GLN:HG2	1.85	0.57
1:A:558:LEU:HB3	1:A:561:GLN:CG	2.34	0.57
1:A:293:ILE:HA	1:A:342:LEU:HD11	1.87	0.56
1:D:507:LYS:NZ	2:H:558:SEP:O2P	2.38	0.56
1:D:523:ARG:HG2	1:D:524:ILE:N	2.20	0.56
1:D:232:GLU:HB2	1:D:243:PHE:HB3	1.88	0.56
1:D:520:ASN:O	1:D:524:ILE:HG13	2.06	0.56
1:A:114:ILE:HD11	1:A:156:TYR:CD2	2.41	0.56
1:B:114:ILE:HD11	1:B:156:TYR:CD2	2.40	0.56
1:D:522:MET:CE	1:D:529:GLY:HA3	2.36	0.55
1:C:395:PRO:HA	1:C:398:ILE:HD12	1.87	0.55
1:D:52:ILE:HG12	1:D:73:MET:HE1	1.89	0.55
1:D:489:ILE:HG23	1:D:501:ILE:HG12	1.90	0.54
1:C:76:ALA:HB3	1:C:116:LEU:HD21	1.90	0.54
1:B:293:ILE:HA	1:B:342:LEU:HD11	1.90	0.53
1:B:510:TYR:O	1:B:512:PRO:HD3	2.09	0.53
1:C:498:VAL:HG21	1:C:532:PHE:HB2	1.89	0.53
1:D:49:GLN:HA	1:D:66:ILE:H	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:ASP:OD1	1:D:396:ASP:N	2.37	0.53
1:A:520:ASN:OD1	1:A:523:ARG:NH2	2.42	0.52
1:A:545:ASP:HB3	1:A:548:GLN:HB2	1.92	0.52
1:B:551:ASP:O	1:B:555:GLU:HG3	2.10	0.52
1:C:168:THR:HG23	1:C:181:MET:HG2	1.92	0.52
1:A:407:GLN:H	1:A:411:THR:HG22	1.75	0.52
1:D:114:ILE:HD11	1:D:156:TYR:CD2	2.44	0.52
1:D:467:VAL:HG21	1:D:478:VAL:HG21	1.92	0.52
1:D:560:GLN:HG2	1:D:561:GLN:HG2	1.92	0.51
1:B:52:ILE:HG12	1:B:73:MET:HE1	1.93	0.51
1:A:395:PRO:HA	1:A:398:ILE:HD12	1.91	0.51
1:C:551:ASP:O	1:C:555:GLU:HG3	2.10	0.51
1:C:490:GLN:O	1:C:494:GLU:HG2	2.10	0.51
1:B:520:ASN:HA	1:B:523:ARG:NH1	2.26	0.51
1:B:168:THR:HG23	1:B:181:MET:HG2	1.93	0.50
1:B:12:HIS:NE2	1:B:326:SER:OG	2.39	0.50
1:B:114:ILE:HD11	1:B:156:TYR:HD2	1.76	0.50
1:B:498:VAL:HA	1:B:501:ILE:HD12	1.93	0.50
1:D:106:ASP:OD1	1:D:106:ASP:N	2.42	0.50
1:C:114:ILE:HD11	1:C:156:TYR:CD2	2.47	0.49
1:C:304:PHE:HD1	1:C:305:VAL:HG13	1.77	0.49
1:C:496:GLY:O	1:C:528:GLN:NE2	2.42	0.49
1:B:486:ASN:HD22	1:B:486:ASN:H	1.60	0.49
1:D:168:THR:HG23	1:D:181:MET:HG2	1.95	0.49
1:A:114:ILE:HD11	1:A:156:TYR:HD2	1.77	0.48
1:D:522:MET:HG3	1:D:552:VAL:CG1	2.43	0.48
1:B:435:LEU:O	1:B:438:PRO:HD2	2.13	0.48
1:C:446:GLN:HG2	1:C:447:LEU:N	2.27	0.48
1:D:86:LYS:O	1:D:103:THR:HG23	2.13	0.48
1:B:12:HIS:CD2	1:B:326:SER:HG	2.32	0.48
1:D:184:TYR:OH	1:D:189:LYS:HG2	2.14	0.48
1:B:12:HIS:HE1	1:B:309:HIS:HE1	1.62	0.48
1:B:546:ILE:O	1:B:549:ILE:HG12	2.14	0.48
1:A:304:PHE:HD1	1:A:305:VAL:HG13	1.79	0.48
1:D:395:PRO:HA	1:D:398:ILE:HD12	1.96	0.48
1:A:209:ASN:OD1	1:A:241:GLN:HG2	2.14	0.47
1:D:498:VAL:HG21	1:D:532:PHE:HB2	1.95	0.47
1:D:518:LEU:O	1:D:522:MET:N	2.36	0.47
1:A:114:ILE:HG12	1:A:120:ALA:HB2	1.96	0.47
1:B:491:CYS:O	1:B:495:THR:OG1	2.33	0.47
1:B:463:LEU:O	1:B:467:VAL:HG22	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:GLY:HA2	1:C:220:VAL:HB	1.97	0.47
1:C:518:LEU:O	1:C:522:MET:HG2	2.15	0.47
1:B:476:LEU:HD23	2:F:565:PRO:HD3	1.97	0.47
1:D:257:GLN:O	1:D:258:ASN:HB2	2.15	0.47
1:A:342:LEU:HD22	1:A:344:ASN:HB2	1.97	0.46
1:A:369:ASN:HA	1:A:400:ARG:HH12	1.81	0.46
1:B:436:CYS:O	1:B:439:VAL:HG12	2.15	0.46
1:B:462:GLU:HA	1:B:465:ASP:OD2	2.15	0.46
1:A:551:ASP:O	1:A:555:GLU:HG3	2.15	0.46
1:B:485:PRO:HB2	1:B:510:TYR:CD2	2.51	0.46
1:A:421:LEU:HB3	1:A:427:LEU:HD21	1.96	0.46
1:A:6:PRO:HB2	1:A:334:ILE:HD12	1.98	0.46
1:A:196:GLY:HA2	1:A:220:VAL:HB	1.96	0.46
1:A:451:TRP:HB3	1:A:457:LEU:CD2	2.45	0.46
1:A:485:PRO:HB2	1:A:510:TYR:CD2	2.51	0.46
1:D:550:VAL:HG13	1:D:562:CYS:SG	2.56	0.46
1:B:196:GLY:HA2	1:B:220:VAL:HB	1.97	0.46
1:B:496:GLY:O	1:B:528:GLN:NE2	2.48	0.46
1:A:102:HIS:CD2	1:A:137:GLN:HG3	2.51	0.46
1:A:51:VAL:HG22	1:A:63:ARG:HG2	1.98	0.45
1:B:95:MET:C	1:B:96:LYS:HG3	2.36	0.45
1:C:114:ILE:HG12	1:C:120:ALA:HB2	1.98	0.45
1:D:114:ILE:HD11	1:D:156:TYR:HD2	1.81	0.45
1:D:545:ASP:HB3	1:D:548:GLN:HB2	1.98	0.45
1:D:507:LYS:HG2	2:H:559:LEU:HD21	1.97	0.45
1:B:49:GLN:HA	1:B:66:ILE:H	1.82	0.45
1:A:546:ILE:O	1:A:549:ILE:HG12	2.16	0.45
1:D:173:GLN:HB2	1:D:178:VAL:HG21	1.99	0.45
1:B:251:PHE:HD2	1:B:295:MET:HE1	1.82	0.45
1:B:450:LYS:O	1:B:454:GLU:HG3	2.17	0.45
1:D:440:LEU:HD13	1:D:470:VAL:HG21	1.98	0.45
1:C:95:MET:C	1:C:96:LYS:HG3	2.37	0.44
1:D:45:GLY:O	1:D:46:GLU:HB2	2.16	0.44
1:D:538:GLN:OE1	1:D:540:GLU:HG2	2.17	0.44
1:A:440:LEU:HD11	1:A:467:VAL:HG12	1.98	0.44
1:C:173:GLN:HB2	1:C:178:VAL:HG21	1.98	0.44
1:A:541:GLU:HG2	1:A:541:GLU:O	2.17	0.44
1:C:342:LEU:HD22	1:C:344:ASN:HB2	1.98	0.44
1:D:522:MET:HG3	1:D:552:VAL:HG12	2.00	0.44
1:A:95:MET:C	1:A:96:LYS:HG3	2.37	0.44
1:A:281:TYR:HA	1:A:297:ARG:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:531:GLN:O	1:D:535:MET:HG3	2.18	0.44
1:B:100:LYS:HE2	1:B:134:GLY:O	2.18	0.44
1:B:536:LEU:HA	1:B:543:LEU:HB2	2.00	0.44
1:C:102:HIS:CD2	1:C:137:GLN:HG3	2.53	0.44
1:D:69:ASP:N	1:D:83:LYS:O	2.48	0.44
1:C:59:SER:O	1:C:61:PRO:HD3	2.18	0.43
1:B:102:HIS:CD2	1:B:137:GLN:HG3	2.53	0.43
1:B:514:TRP:CZ3	1:B:532:PHE:HZ	2.36	0.43
1:B:517:LEU:HD23	1:B:517:LEU:HA	1.86	0.43
1:D:176:ARG:HA	1:D:176:ARG:HD2	1.65	0.43
1:A:66:ILE:HG21	1:A:82:LEU:HD22	2.00	0.43
1:D:95:MET:C	1:D:96:LYS:HG3	2.37	0.43
1:C:100:LYS:HE2	1:C:134:GLY:O	2.19	0.43
1:C:114:ILE:HD11	1:C:156:TYR:HD2	1.83	0.43
1:D:524:ILE:HG13	1:D:524:ILE:H	1.53	0.43
1:B:369:ASN:HA	1:B:400:ARG:HH12	1.84	0.43
1:C:62:ILE:HG21	1:C:64:ARG:HE	1.83	0.43
1:C:335:ILE:HB	1:C:336:PRO:HD3	2.01	0.43
1:A:266:ILE:HG12	1:A:273:VAL:HG22	1.99	0.43
1:B:507:LYS:HE2	1:B:507:LYS:HB2	1.85	0.43
1:B:550:VAL:O	1:B:554:MET:HG2	2.19	0.43
1:C:283:HIS:HB3	1:C:285:TYR:CE1	2.53	0.43
1:B:411:THR:HG23	1:C:446:GLN:HG3	2.01	0.42
1:C:339:THR:O	1:C:343:GLN:HA	2.19	0.42
1:D:196:GLY:HA2	1:D:220:VAL:HB	2.01	0.42
1:A:47:GLN:HE21	1:A:47:GLN:HB3	1.58	0.42
1:B:114:ILE:HG12	1:B:120:ALA:HB2	2.01	0.42
1:C:433:LEU:HD21	1:C:437:ARG:HH12	1.84	0.42
1:D:407:GLN:O	1:D:409:GLY:N	2.52	0.42
1:C:114:ILE:HD13	1:C:114:ILE:HA	1.80	0.42
1:D:342:LEU:HD22	1:D:344:ASN:HB2	2.02	0.42
1:B:520:ASN:HA	1:B:523:ARG:HH11	1.83	0.42
1:A:345:PRO:HG2	1:B:223:GLN:HA	2.02	0.42
1:A:498:VAL:HA	1:A:501:ILE:HD12	2.00	0.42
1:A:407:GLN:N	1:A:411:THR:HG22	2.34	0.42
1:C:427:LEU:O	1:C:458:GLU:HB2	2.20	0.42
1:C:293:ILE:O	1:C:294:TYR:HB3	2.20	0.42
1:D:117:ASN:HA	1:D:132:MET:SD	2.60	0.42
1:B:232:GLU:HB2	1:B:243:PHE:HB3	2.00	0.42
1:B:519:ARG:NH1	1:B:555:GLU:OE1	2.50	0.42
1:C:460:SER:OG	1:C:461:GLU:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ILE:HG21	1:B:82:LEU:HD22	2.02	0.41
1:C:106:ASP:OD1	1:C:106:ASP:N	2.39	0.41
1:C:513:ASP:HB3	1:C:516:PHE:HB3	2.02	0.41
1:B:342:LEU:HD22	1:B:344:ASN:HB2	2.01	0.41
1:A:476:LEU:HD23	2:E:565:PRO:HD3	2.02	0.41
1:A:512:PRO:HD2	1:A:514:TRP:CE2	2.55	0.41
1:C:71:ALA:HB1	1:C:80:ILE:HD11	2.02	0.41
1:D:339:THR:O	1:D:343:GLN:HA	2.20	0.41
1:A:283:HIS:HB3	1:A:285:TYR:CE2	2.55	0.41
1:B:257:GLN:O	1:B:258:ASN:HB2	2.21	0.41
1:D:335:ILE:HB	1:D:336:PRO:HD3	2.01	0.41
1:A:339:THR:O	1:A:343:GLN:HA	2.21	0.41
1:A:429:LYS:HD3	1:A:460:SER:HB3	2.01	0.41
1:B:164:TRP:CE2	1:B:233:VAL:HB	2.56	0.41
1:D:419:GLY:HA2	1:D:422:LEU:HD12	2.02	0.41
1:C:117:ASN:HA	1:C:132:MET:HB3	2.03	0.41
1:C:164:TRP:CH2	1:C:234:GLY:HA3	2.56	0.41
1:B:335:ILE:HB	1:B:336:PRO:HD3	2.03	0.41
1:A:45:GLY:O	1:A:46:GLU:HB2	2.20	0.41
1:D:100:LYS:HZ1	1:D:136:SER:H	1.68	0.41
2:G:566:LEU:HA	2:G:566:LEU:HD23	1.88	0.41
1:A:114:ILE:HD13	1:A:114:ILE:HA	1.75	0.41
1:A:236:PRO:HG3	1:A:242:PRO:HB3	2.03	0.41
1:B:137:GLN:HG3	1:B:138:PRO:HD2	2.03	0.40
1:C:445:LYS:HA	1:C:448:LEU:HD23	2.03	0.40
1:B:6:PRO:HB2	1:B:334:ILE:HD12	2.03	0.40
1:B:197:HIS:CB	1:B:261:PRO:HG2	2.47	0.40
1:B:339:THR:O	1:B:343:GLN:HA	2.22	0.40
1:D:546:ILE:H	1:D:546:ILE:HG12	1.39	0.40
1:A:129:HIS:CD2	1:A:141:MET:HG3	2.57	0.40
1:B:9:PHE:CZ	1:B:325:LEU:HD22	2.56	0.40
1:B:513:ASP:HB3	1:B:516:PHE:HB3	2.04	0.40
1:D:114:ILE:HD13	1:D:114:ILE:HA	1.79	0.40
1:D:352:ALA:HB1	1:D:360:ALA:HB2	2.02	0.40
1:D:485:PRO:HB2	1:D:510:TYR:CD2	2.56	0.40
1:A:335:ILE:HB	1:A:336:PRO:HD3	2.02	0.40
1:D:235:THR:HA	1:D:236:PRO:HD3	1.98	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	570/574 (99%)	545 (96%)	25 (4%)	0	100	100
1	B	563/574 (98%)	532 (94%)	31 (6%)	0	100	100
1	C	544/574 (95%)	518 (95%)	26 (5%)	0	100	100
1	D	569/574 (99%)	538 (95%)	31 (5%)	0	100	100
2	E	15/18 (83%)	14 (93%)	1 (7%)	0	100	100
2	F	15/18 (83%)	14 (93%)	1 (7%)	0	100	100
2	G	15/18 (83%)	14 (93%)	1 (7%)	0	100	100
2	H	15/18 (83%)	15 (100%)	0	0	100	100
All	All	2306/2368 (97%)	2190 (95%)	116 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	486/494 (98%)	433 (89%)	53 (11%)	6	25
1	B	477/494 (97%)	427 (90%)	50 (10%)	7	26
1	C	469/494 (95%)	426 (91%)	43 (9%)	9	33
1	D	477/494 (97%)	428 (90%)	49 (10%)	7	27
2	E	14/16 (88%)	12 (86%)	2 (14%)	3	14
2	F	13/16 (81%)	11 (85%)	2 (15%)	2	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	13/16 (81%)	11 (85%)	2 (15%)	2 11
2	H	14/16 (88%)	11 (79%)	3 (21%)	1 4
All	All	1963/2040 (96%)	1759 (90%)	204 (10%)	7 27

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	5	LEU
1	A	10	GLN
1	A	12	HIS
1	A	13	LEU
1	A	47	GLN
1	A	69	ASP
1	A	82	LEU
1	A	104	MET
1	A	107	ASP
1	A	111	TRP
1	A	116	LEU
1	A	117	ASN
1	A	118	THR
1	A	137	GLN
1	A	161	LYS
1	A	163	LYS
1	A	164	TRP
1	A	176	ARG
1	A	188	ARG
1	A	189	LYS
1	A	209	ASN
1	A	248	VAL
1	A	255	GLU
1	A	284	LEU
1	A	309	HIS
1	A	326	SER
1	A	334	ILE
1	A	351	MET
1	A	362	GLU
1	A	396	ASP
1	A	411	THR
1	A	414	LEU
1	A	420	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	422	LEU
1	A	445	LYS
1	A	456	LYS
1	A	457	LEU
1	A	459	CYS
1	A	461	GLU
1	A	465	ASP
1	A	466	LEU
1	A	468	LYS
1	A	477	SER
1	A	480	LEU
1	A	484	VAL
1	A	494	GLU
1	A	518	LEU
1	A	527	ASP
1	A	541	GLU
1	A	560	GLN
1	A	561	GLN
1	A	568	ASP
1	B	3	GLN
1	B	5	LEU
1	B	10	GLN
1	B	13	LEU
1	B	69	ASP
1	B	82	LEU
1	B	98	LYS
1	B	104	MET
1	B	107	ASP
1	B	111	TRP
1	B	118	THR
1	B	137	GLN
1	B	154	ILE
1	B	163	LYS
1	B	176	ARG
1	B	188	ARG
1	B	189	LYS
1	B	231	ILE
1	B	255	GLU
1	B	262	VAL
1	B	284	LEU
1	B	351	MET
1	B	362	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	411	THR
1	B	416	GLN
1	B	427	LEU
1	B	431	GLU
1	B	439	VAL
1	B	440	LEU
1	B	446	GLN
1	B	457	LEU
1	B	458	GLU
1	B	469	SER
1	B	477	SER
1	B	480	LEU
1	B	484	VAL
1	B	495	THR
1	B	507	LYS
1	B	518	LEU
1	B	519	ARG
1	B	531	GLN
1	B	539	ASP
1	B	541	GLU
1	B	546	ILE
1	B	557	ASN
1	B	558	LEU
1	B	559	ILE
1	B	560	GLN
1	B	561	GLN
1	B	568	ASP
1	C	3	GLN
1	C	5	LEU
1	C	10	GLN
1	C	12	HIS
1	C	13	LEU
1	C	69	ASP
1	C	82	LEU
1	C	98	LYS
1	C	104	MET
1	C	107	ASP
1	C	111	TRP
1	C	116	LEU
1	C	118	THR
1	C	137	GLN
1	C	154	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	163	LYS
1	C	164	TRP
1	C	170	ILE
1	C	176	ARG
1	C	188	ARG
1	C	189	LYS
1	C	209	ASN
1	C	255	GLU
1	C	284	LEU
1	C	296	ASN
1	C	351	MET
1	C	362	GLU
1	C	446	GLN
1	C	447	LEU
1	C	461	GLU
1	C	463	LEU
1	C	477	SER
1	C	480	LEU
1	C	484	VAL
1	C	495	THR
1	C	497	GLN
1	C	498	VAL
1	C	518	LEU
1	C	524	ILE
1	C	525	SER
1	C	531	GLN
1	C	546	ILE
1	C	568	ASP
1	D	3	GLN
1	D	5	LEU
1	D	10	GLN
1	D	12	HIS
1	D	13	LEU
1	D	69	ASP
1	D	82	LEU
1	D	98	LYS
1	D	104	MET
1	D	107	ASP
1	D	111	TRP
1	D	116	LEU
1	D	118	THR
1	D	132	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	154	ILE
1	D	163	LYS
1	D	164	TRP
1	D	188	ARG
1	D	189	LYS
1	D	255	GLU
1	D	282	ILE
1	D	284	LEU
1	D	349	LEU
1	D	362	GLU
1	D	396	ASP
1	D	424	GLN
1	D	427	LEU
1	D	433	LEU
1	D	440	LEU
1	D	441	GLN
1	D	448	LEU
1	D	452	LEU
1	D	457	LEU
1	D	461	GLU
1	D	465	ASP
1	D	477	SER
1	D	480	LEU
1	D	484	VAL
1	D	498	VAL
1	D	507	LYS
1	D	508	VAL
1	D	518	LEU
1	D	522	MET
1	D	524	ILE
1	D	543	LEU
1	D	546	ILE
1	D	558	LEU
1	D	561	GLN
1	D	568	ASP
2	E	559	LEU
2	E	564	ASP
2	F	559	LEU
2	F	564	ASP
2	G	559	LEU
2	G	564	ASP
2	H	559	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	564	ASP
2	H	567	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	47	GLN
1	A	102	HIS
1	A	486	ASN
1	B	49	GLN
1	B	102	HIS
1	B	309	HIS
1	B	528	GLN
1	B	561	GLN
1	C	17	ASN
1	C	102	HIS
1	D	17	ASN
1	D	49	GLN
1	D	426	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

4 non-standard protein/DNA/RNA residues 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	SEP	G	558	2	8,9,10	1.46	1 (12%)	8,12,14	2.13	2 (25%)
2	SEP	E	558	2	8,9,10	1.46	1 (12%)	8,12,14	2.11	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SEP	F	558	2	8,9,10	1.46	1 (12%)	8,12,14	2.08	2 (25%)
2	SEP	H	558	2	8,9,10	1.49	1 (12%)	8,12,14	2.28	2 (25%)

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	SEP	G	558	2	-	1/5/8/10	-
2	SEP	E	558	2	-	1/5/8/10	-
2	SEP	F	558	2	-	1/5/8/10	-
2	SEP	H	558	2	-	1/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	558	SEP	P-O1P	3.25	1.61	1.50
2	G	558	SEP	P-O1P	3.22	1.60	1.50
2	E	558	SEP	P-O1P	3.21	1.60	1.50
2	F	558	SEP	P-O1P	3.17	1.60	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	558	SEP	OG-CB-CA	4.59	112.61	108.14
2	G	558	SEP	OG-CB-CA	4.14	112.17	108.14
2	H	558	SEP	P-OG-CB	-4.07	107.08	118.30
2	E	558	SEP	OG-CB-CA	4.05	112.09	108.14
2	F	558	SEP	OG-CB-CA	3.97	112.01	108.14
2	E	558	SEP	P-OG-CB	-3.92	107.49	118.30
2	G	558	SEP	P-OG-CB	-3.89	107.59	118.30
2	F	558	SEP	P-OG-CB	-3.85	107.69	118.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	558	SEP	N-CA-CB-OG
2	F	558	SEP	N-CA-CB-OG
2	G	558	SEP	N-CA-CB-OG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	H	558	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	558	SEP	1	0

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	443:GLY	C	444:ARG	N	3.27

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	572/574 (99%)	-0.16	0 100 100	50, 92, 150, 189	0
1	B	567/574 (98%)	-0.07	7 (1%) 79 61	56, 114, 182, 213	0
1	C	554/574 (96%)	0.17	21 (3%) 40 20	73, 139, 215, 245	0
1	D	571/574 (99%)	0.02	9 (1%) 72 51	74, 124, 171, 207	0
2	E	17/18 (94%)	-0.21	0 100 100	114, 147, 167, 169	0
2	F	17/18 (94%)	0.18	1 (5%) 22 10	175, 195, 208, 210	0
2	G	17/18 (94%)	0.19	1 (5%) 22 10	182, 191, 240, 251	0
2	H	17/18 (94%)	0.20	1 (5%) 22 10	138, 167, 206, 208	0
All	All	2332/2368 (98%)	-0.01	40 (1%) 70 49	50, 119, 200, 251	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	456	LYS	4.5
2	G	563	PHE	4.4
1	D	18	LEU	4.4
1	C	454	GLU	4.2
1	D	50	VAL	4.0
1	D	495	THR	3.1
1	B	392	LEU	3.1
1	C	493	ALA	3.0
1	C	451	TRP	3.0
1	B	85	GLY	3.0
1	B	498	VAL	2.9
1	C	211	GLU	2.9
1	C	417	TYR	2.6
1	B	454	GLU	2.5
1	C	469	SER	2.5
1	C	470	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	88	LEU	2.5
1	C	372	PHE	2.5
1	C	15	LEU	2.4
1	C	544	ALA	2.4
2	F	567	LEU	2.4
1	C	418	PHE	2.4
1	D	539	ASP	2.4
1	B	418	PHE	2.4
1	D	457	LEU	2.3
1	B	501	ILE	2.3
1	C	82	LEU	2.3
2	H	552	SER	2.3
1	C	435	LEU	2.2
1	C	459	CYS	2.2
1	C	373	ALA	2.2
1	D	411	THR	2.2
1	C	505	ALA	2.1
1	C	457	LEU	2.1
1	D	408	PRO	2.1
1	C	484	VAL	2.1
1	D	20	ILE	2.1
1	C	460	SER	2.1
1	C	119	VAL	2.0
1	B	514	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	SEP	F	558	10/11	0.87	0.08	195,200,210,213	0
2	SEP	H	558	10/11	0.88	0.15	172,182,188,190	0
2	SEP	E	558	10/11	0.91	0.09	134,148,157,158	0
2	SEP	G	558	10/11	0.93	0.08	184,190,200,203	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.