Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 01:42 PM EDT

PDB ID	:	2I04
Title	:	X-ray crystal structure of MAGI-1 PDZ1 bound to the C-terminal peptide of HPV18 E6
Authors	:	Chen, X.S.; Zhang, Y.; Dasgupta, J.; Banks, L.; Thomas, M.
Deposited on	:	2006-08-09
Resolution	:	2.15 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:

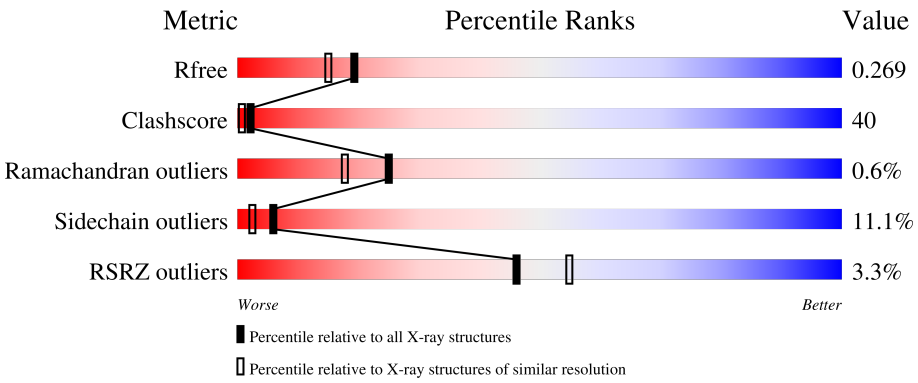
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	85	2%, 49%, 31%, 19%, •
1	B	85	2%, 48%, 39%, 11%, •
2	C	7	14%, 14%, 43%, 14%, 29%
2	D	7	14%, 14%, 71%, 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1608 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 Membrane-associated guanylate kinase, WW and PDZ domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	85	635	400	109	123	3	0	0	0
1	B	85	635	400	109	123	3	0	0	0

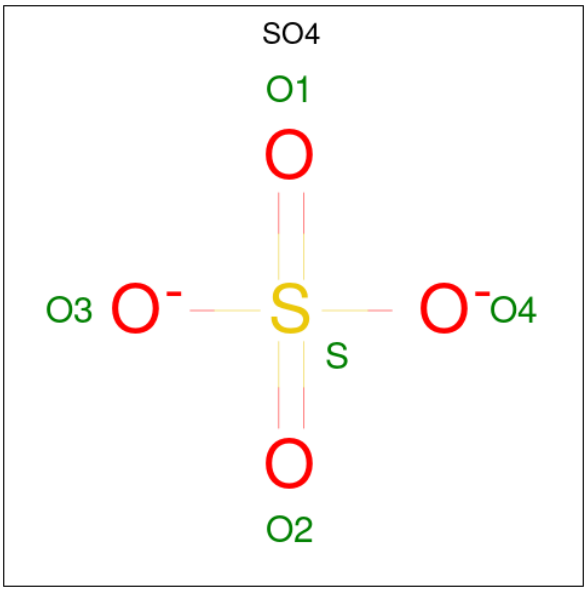
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	450	SER	-	CLONING ARTIFACT	UNP Q6RHR9
B	450	SER	-	CLONING ARTIFACT	UNP Q6RHR9

- Molecule 2 is a protein called peptide E6.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	5	44	25	9	10	0	0	0
2	D	7	60	34	14	12	0	0	0

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



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

- Molecule 4 is water.

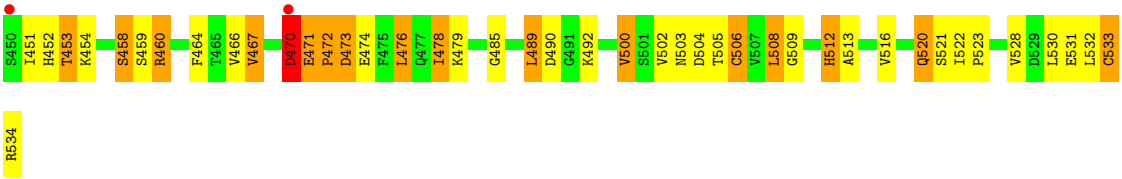
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	101	Total O 101 101	0	0
4	C	9	Total O 9 9	0	0
4	B	98	Total O 98 98	0	0
4	D	16	Total O 16 16	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

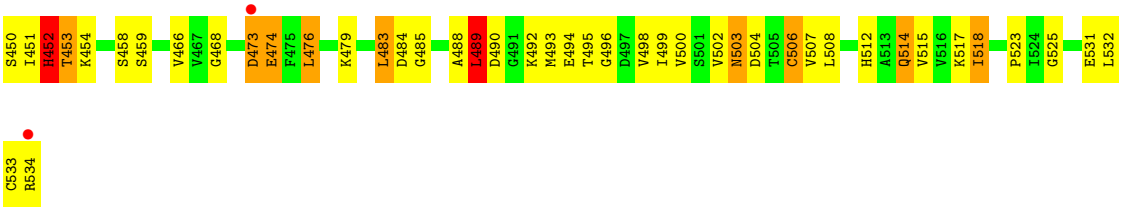
• Molecule 1: Membrane-associated guanylate kinase, WW and PDZ domain-containing protein 1

Chain A:



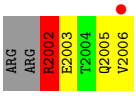
• Molecule 1: Membrane-associated guanylate kinase, WW and PDZ domain-containing protein 1

Chain B:



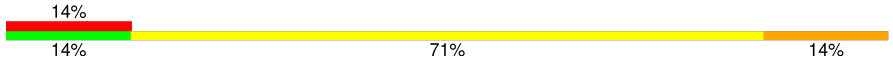
• Molecule 2: peptide E6

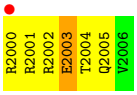
Chain C:



• Molecule 2: peptide E6

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.96Å 27.61Å 59.52Å 90.00° 105.42° 90.00°	Depositor
Resolution (Å)	28.69 – 2.15 47.20 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.4 (28.69-2.15) 97.5 (47.20-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	17.31 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.269 0.215 , 0.269	Depositor DCC
R_{free} test set	516 reflections (5.55%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	1608	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.30	14/644 (2.2%)	1.32	15/869 (1.7%)
1	B	1.10	11/644 (1.7%)	1.17	9/869 (1.0%)
2	C	2.02	2/43 (4.7%)	2.74	5/55 (9.1%)
2	D	2.33	2/59 (3.4%)	2.13	4/76 (5.3%)
All	All	1.31	29/1390 (2.1%)	1.36	33/1869 (1.8%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2003	GLU	C-N	-12.81	1.04	1.34
1	A	471	GLU	C-N	11.69	1.56	1.34
1	B	484	ASP	C-N	11.58	1.53	1.33
2	D	2005	GLN	C-N	-11.04	1.08	1.34
1	A	513	ALA	C-N	9.74	1.56	1.34
2	C	2005	GLN	C-N	-9.67	1.11	1.34
1	A	460	ARG	C-N	9.57	1.50	1.33
1	B	496	GLY	C-N	9.12	1.55	1.34
1	A	520	GLN	C-N	8.43	1.53	1.34
1	A	470	ASP	C-N	-8.34	1.14	1.34
1	A	472	PRO	C-N	8.05	1.52	1.34
1	A	533	CYS	C-N	7.92	1.52	1.34
1	B	459	SER	C-N	7.66	1.51	1.34
1	A	521	SER	C-N	7.48	1.51	1.34
2	C	2002	ARG	C-N	-7.11	1.17	1.34
1	A	532	LEU	C-N	-7.11	1.17	1.34
1	B	488	ALA	C-N	7.02	1.50	1.34
1	B	514	GLN	C-N	6.99	1.50	1.34
1	A	516	VAL	C-N	6.66	1.49	1.34
1	B	506	CYS	C-N	6.62	1.49	1.34
1	B	489	LEU	C-N	6.47	1.49	1.34
1	A	500	VAL	C-N	6.43	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	508	LEU	C-N	-6.40	1.21	1.33
1	A	459	SER	C-N	6.21	1.48	1.34
1	A	478	ILE	C-N	5.95	1.47	1.34
1	B	458	SER	C-N	5.79	1.47	1.34
1	A	458	SER	C-N	5.73	1.47	1.34
1	B	525	GLY	C-N	5.58	1.46	1.34
1	B	495	THR	C-N	5.48	1.43	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	532	LEU	O-C-N	-12.09	103.36	122.70
2	C	2002	ARG	O-C-N	-11.60	104.13	122.70
1	A	532	LEU	CA-C-N	8.86	136.70	117.20
1	A	512	HIS	O-C-N	-8.66	108.85	122.70
1	A	532	LEU	C-N-CA	8.43	142.78	121.70
2	C	2003	GLU	O-C-N	-7.99	109.92	122.70
2	C	2002	ARG	CA-C-N	7.96	134.72	117.20
1	A	513	ALA	O-C-N	7.70	135.02	122.70
1	A	506	CYS	O-C-N	-7.55	110.61	122.70
2	D	2000	ARG	C-N-CA	6.88	138.90	121.70
2	D	2003	GLU	O-C-N	-6.71	111.97	122.70
1	B	451	ILE	O-C-N	-6.65	112.06	122.70
1	A	508	LEU	C-N-CA	6.54	136.03	122.30
1	A	508	LEU	O-C-N	-6.52	112.11	123.20
1	B	489	LEU	O-C-N	6.48	133.07	122.70
1	A	512	HIS	CA-C-N	6.10	130.62	117.20
1	A	512	HIS	C-N-CA	6.02	136.74	121.70
1	B	503	ASN	O-C-N	6.02	132.33	122.70
2	D	2003	GLU	C-N-CA	5.89	136.43	121.70
1	B	452	HIS	O-C-N	-5.75	113.51	122.70
1	A	506	CYS	C-N-CA	5.71	135.96	121.70
2	C	2002	ARG	C-N-CA	5.58	135.64	121.70
1	A	459	SER	O-C-N	5.57	131.61	122.70
1	B	514	GLN	O-C-N	5.53	131.55	122.70
1	A	513	ALA	CA-C-N	-5.47	105.16	117.20
1	B	488	ALA	O-C-N	-5.44	114.00	122.70
2	D	2004	THR	O-C-N	-5.38	114.08	122.70
2	C	2003	GLU	CA-C-N	5.24	128.72	117.20
1	A	508	LEU	CA-C-N	5.23	126.66	116.20
1	B	489	LEU	CA-C-N	-5.22	105.72	117.20
1	B	503	ASN	CA-C-N	-5.13	105.91	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	506	CYS	CA-C-N	5.13	128.48	117.20
1	B	483	LEU	O-C-N	-5.01	114.69	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	635	0	637	71	0
1	B	635	0	640	45	0
2	C	44	0	39	12	0
2	D	60	0	55	2	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
4	A	101	0	0	11	0
4	B	98	0	0	9	1
4	C	9	0	0	0	0
4	D	16	0	0	2	0
All	All	1608	0	1371	107	1

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 40.

All (107) 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:470:ASP:HA	2:C:2002:ARG:NH2	1.45	1.31
1:A:520:GLN:HG3	4:A:2311:HOH:O	1.38	1.19
1:A:472:PRO:HD3	4:A:2328:HOH:O	1.47	1.14
1:A:470:ASP:CA	2:C:2002:ARG:NH2	2.13	1.09
1:A:470:ASP:OD1	1:A:474:GLU:OE2	1.77	1.02
1:A:470:ASP:CG	2:C:2002:ARG:NH2	2.15	1.00
1:B:523:PRO:HG3	4:B:2312:HOH:O	1.58	1.00
4:A:2311:HOH:O	2:C:2006:VAL:HG12	1.61	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:LYS:HD2	4:B:2322:HOH:O	1.68	0.93
1:A:453:THR:HG23	1:A:492:LYS:HE2	1.48	0.92
1:A:474:GLU:HG3	1:B:473:ASP:HB2	1.52	0.90
1:A:506:CYS:HG	1:B:533:CYS:HG	1.03	0.87
1:A:470:ASP:HA	2:C:2002:ARG:HH22	1.31	0.87
1:B:502:VAL:HG11	1:B:518:ILE:HD11	1.58	0.85
1:A:470:ASP:OD2	2:C:2002:ARG:NH2	2.09	0.85
1:A:466:VAL:HB	1:A:476:LEU:CD2	2.08	0.83
1:B:494:GLU:HG2	1:B:534:ARG:NH2	1.94	0.82
1:A:470:ASP:CG	2:C:2002:ARG:HH21	1.79	0.82
1:A:522:ILE:HD13	1:A:528:VAL:CG1	2.09	0.82
1:A:534:ARG:OXT	4:A:2139:HOH:O	1.97	0.82
1:A:470:ASP:CB	2:C:2002:ARG:NH2	2.44	0.80
1:A:476:LEU:HD12	4:A:2071:HOH:O	1.82	0.77
1:B:493:MET:HG2	1:B:532:LEU:HD11	1.66	0.77
1:A:522:ILE:HD13	1:A:528:VAL:HG13	1.67	0.77
1:A:506:CYS:CB	1:B:533:CYS:HG	1.99	0.76
1:B:454:LYS:HD2	4:B:2229:HOH:O	1.87	0.75
1:A:470:ASP:CA	2:C:2002:ARG:HH21	2.00	0.73
1:B:468:GLY:O	1:B:512:HIS:HB2	1.89	0.72
1:B:466:VAL:HB	1:B:476:LEU:HD23	1.71	0.71
1:A:466:VAL:HB	1:A:476:LEU:HD22	1.72	0.71
1:B:485:GLY:O	1:B:489:LEU:HD22	1.90	0.70
1:A:470:ASP:CB	2:C:2002:ARG:HH22	2.05	0.70
1:B:514:GLN:O	1:B:518:ILE:HG23	1.93	0.69
1:A:485:GLY:O	1:A:489:LEU:HD12	1.94	0.67
1:A:470:ASP:CA	2:C:2002:ARG:HH22	1.94	0.66
1:A:467:VAL:HG21	1:A:479:LYS:HD2	1.77	0.66
1:A:460:ARG:HD3	4:A:2086:HOH:O	1.96	0.65
1:B:502:VAL:CG1	1:B:518:ILE:HD11	2.25	0.65
1:A:453:THR:HG21	1:A:492:LYS:HB2	1.79	0.65
1:A:453:THR:HG21	1:A:490:ASP:OD1	1.96	0.65
1:A:458:SER:HB2	3:A:901:SO4:O3	1.98	0.64
1:A:471:GLU:OE2	1:A:473:ASP:HB2	1.98	0.64
1:A:467:VAL:CG2	1:A:479:LYS:HB2	2.27	0.63
1:A:470:ASP:HB2	1:A:474:GLU:OE1	1.99	0.63
1:A:522:ILE:CD1	1:A:528:VAL:CG1	2.77	0.63
1:B:493:MET:HG2	1:B:532:LEU:CD1	2.28	0.63
1:A:479:LYS:NZ	4:A:2314:HOH:O	2.32	0.62
1:A:502:VAL:O	1:A:505:THR:HG22	2.02	0.59
1:B:452:HIS:HB2	4:B:2171:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:THR:CG2	1:B:492:LYS:HB2	2.33	0.59
1:A:533:CYS:HG	1:B:506:CYS:HG	1.51	0.59
1:A:474:GLU:CG	1:B:473:ASP:HB2	2.28	0.57
2:D:2002:ARG:NH1	4:D:2226:HOH:O	2.37	0.56
1:A:503:ASN:HD21	1:A:528:VAL:HG12	1.71	0.56
1:B:453:THR:HG21	1:B:492:LYS:HB2	1.87	0.55
1:A:467:VAL:HG22	1:A:479:LYS:HB2	1.88	0.55
1:A:451:ILE:CD1	1:A:534:ARG:CZ	2.84	0.55
1:A:522:ILE:HD13	1:A:528:VAL:HG11	1.89	0.54
1:A:453:THR:CG2	1:A:492:LYS:HB2	2.37	0.54
1:A:508:LEU:HD13	1:B:498:VAL:HG11	1.90	0.54
1:B:476:LEU:HD11	1:B:512:HIS:HA	1.90	0.53
1:A:472:PRO:HG2	4:A:2306:HOH:O	2.09	0.53
1:A:470:ASP:HB2	1:A:474:GLU:CD	2.30	0.52
2:D:2003:GLU:OE2	4:D:2031:HOH:O	2.19	0.52
1:A:503:ASN:O	1:A:504:ASP:HB2	2.09	0.52
1:B:453:THR:HG22	1:B:492:LYS:CE	2.39	0.51
1:B:523:PRO:CG	4:B:2312:HOH:O	2.35	0.51
1:A:502:VAL:HG22	1:A:530:LEU:CD1	2.41	0.51
1:B:503:ASN:O	1:B:504:ASP:HB3	2.12	0.50
1:A:453:THR:CG2	1:A:490:ASP:OD1	2.60	0.50
1:B:499:ILE:HG22	1:B:507:VAL:HG21	1.93	0.50
1:A:452:HIS:HB3	4:A:2308:HOH:O	2.12	0.50
1:A:512:HIS:CE1	2:C:2002:ARG:HG3	2.47	0.49
1:B:453:THR:HG21	1:B:490:ASP:OD1	2.13	0.49
1:A:472:PRO:O	1:A:509:GLY:HA2	2.12	0.49
1:B:512:HIS:O	1:B:515:VAL:HG12	2.13	0.49
1:A:503:ASN:ND2	1:A:528:VAL:HG12	2.28	0.49
1:B:453:THR:HG22	1:B:492:LYS:HE3	1.94	0.49
1:A:460:ARG:HE	1:A:460:ARG:HB2	1.48	0.48
1:A:522:ILE:CD1	1:A:528:VAL:HG11	2.43	0.48
1:B:476:LEU:CD2	1:B:515:VAL:HG11	2.45	0.47
1:A:453:THR:HG23	1:A:492:LYS:CE	2.34	0.47
1:A:506:CYS:CB	1:B:533:CYS:SG	3.02	0.47
1:A:464:PHE:CD2	1:A:478:ILE:HD12	2.50	0.47
1:A:452:HIS:CE1	1:A:531:GLU:CD	2.89	0.46
1:A:467:VAL:HG21	1:A:479:LYS:CD	2.43	0.45
1:B:453:THR:HG23	1:B:492:LYS:HD2	1.97	0.45
1:A:451:ILE:HD11	1:A:534:ARG:CZ	2.46	0.45
1:B:523:PRO:CD	4:B:2312:HOH:O	2.62	0.45
1:B:474:GLU:N	4:B:2082:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:GLU:HG2	1:B:534:ARG:HH21	1.79	0.45
1:B:517:LYS:CD	4:B:2322:HOH:O	2.42	0.45
1:A:522:ILE:HA	1:A:523:PRO:HD2	1.84	0.45
1:A:506:CYS:HB2	1:B:533:CYS:SG	2.57	0.44
1:A:473:ASP:O	1:B:474:GLU:HA	2.17	0.44
1:A:472:PRO:CG	4:A:2306:HOH:O	2.65	0.44
1:B:476:LEU:HD22	1:B:515:VAL:HG11	2.00	0.43
1:A:454:LYS:HE3	1:A:454:LYS:HB2	1.88	0.42
1:A:452:HIS:CE1	1:A:531:GLU:CG	3.03	0.42
1:A:452:HIS:HE1	1:A:531:GLU:CD	2.23	0.42
1:B:450:SER:N	4:B:2183:HOH:O	2.51	0.42
1:A:454:LYS:HE2	4:A:2123:HOH:O	2.19	0.42
1:A:500:VAL:HG12	1:B:533:CYS:SG	2.60	0.42
1:B:494:GLU:OE2	1:B:534:ARG:CZ	2.68	0.42
1:A:533:CYS:SG	1:B:500:VAL:HG12	2.61	0.40
1:A:506:CYS:HB2	1:B:533:CYS:HG	1.81	0.40
1:B:453:THR:CG2	1:B:490:ASP:OD1	2.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2052:HOH:O	4:B:2094:HOH:O[2_756]	2.05	0.15

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	83/85 (98%)	79 (95%)	3 (4%)	1 (1%)	13 7
1	B	83/85 (98%)	81 (98%)	2 (2%)	0	100 100
2	C	3/7 (43%)	3 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	5/7 (71%)	5 (100%)	0	0	100	100
All	All	174/184 (95%)	168 (97%)	5 (3%)	1 (1%)	25	18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	470	ASP

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	71/72 (99%)	66 (93%)	5 (7%)	15	10
1	B	71/72 (99%)	61 (86%)	10 (14%)	3	1
2	C	5/7 (71%)	4 (80%)	1 (20%)	1	0
2	D	6/7 (86%)	5 (83%)	1 (17%)	2	1
All	All	153/158 (97%)	136 (89%)	17 (11%)	6	2

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	453	THR
1	A	467	VAL
1	A	473	ASP
1	A	476	LEU
1	A	489	LEU
2	C	2002	ARG
1	B	452	HIS
1	B	453	THR
1	B	473	ASP
1	B	474	GLU
1	B	476	LEU
1	B	479	LYS
1	B	483	LEU

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Mol	Chain	Res	Type
1	B	489	LEU
1	B	518	ILE
1	B	531	GLU
2	D	2001	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	452	HIS
1	A	520	GLN
1	B	514	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
3	SO4	A	901	-	4,4,4	0.33	0	6,6,6	0.06	0
3	SO4	B	900	-	4,4,4	0.31	0	6,6,6	0.09	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	SO4	1	0

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	A	2
2	C	2
2	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	532:LEU	C	533:CYS	N	1.17
1	C	2002:ARG	C	2003:GLU	N	1.17
1	A	470:ASP	C	471:GLU	N	1.14
1	C	2005:GLN	C	2006:VAL	N	1.11
1	D	2005:GLN	C	2006:VAL	N	1.08
1	D	2003:GLU	C	2004:THR	N	1.04

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	85/85 (100%)	-0.05	2 (2%)	59	67	10, 20, 41, 53	0
1	B	85/85 (100%)	-0.11	2 (2%)	59	67	12, 20, 39, 46	0
2	C	5/7 (71%)	0.66	1 (20%)	1	1	18, 21, 38, 46	0
2	D	7/7 (100%)	0.26	1 (14%)	2	3	14, 21, 37, 43	0
All	All	182/184 (98%)	-0.05	6 (3%)	46	55	10, 21, 41, 53	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	470	ASP	3.5
2	C	2006	VAL	3.2
1	B	473	ASP	2.8
2	D	2000	ARG	2.5
1	B	534	ARG	2.3
1	A	450	SER	2.2

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, 95th 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	900	5/5	0.95	0.12	42,46,49,49	0
3	SO4	A	901	5/5	0.96	0.13	45,48,52,53	0

6.5 Other polymers (i)

There are no such residues in this entry.