Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 09:52 AM EDT

PDB ID	:	1T3E
Title	:	Structural basis of dynamic glycine receptor clustering
Authors	:	Sola, M.; Bavro, V.N.; Timmins, J.; Franz, T.; Ricard-Blum, S.; Schoehn, G.; Ruigrok, R.W.H.; Paarmann, I.; Saiyed, T.; O'Sullivan, G.A.
Deposited on	:	2004-04-26
Resolution	:	3.25 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:

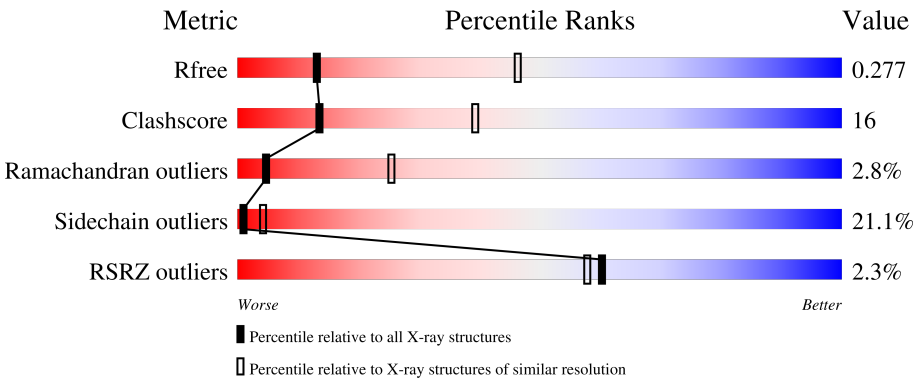
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	421	% 52% 38% 7% • •
1	B	421	3% 53% 34% 8% • •
2	P	49	6% • 90%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	2	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6243 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.

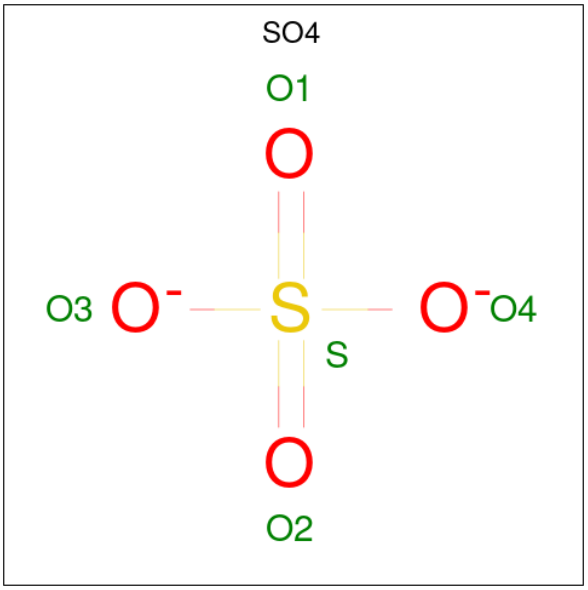
- Molecule 1 is a protein called Gephyrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	412	3117	1966	542	591	18	0	0	0
1	B	405	3064	1933	534	577	20	0	0	0

- Molecule 2 is a protein called 49-mer fragment of Glycine receptor beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	P	5	22	12	5	5	0	0	0

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



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

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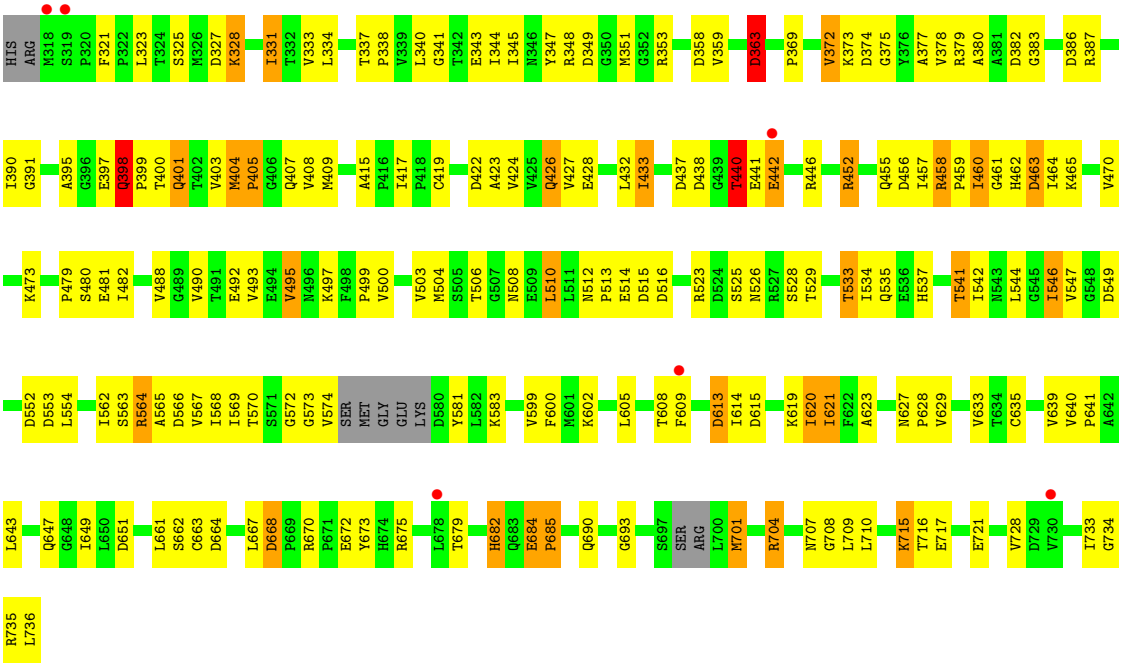
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0

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.

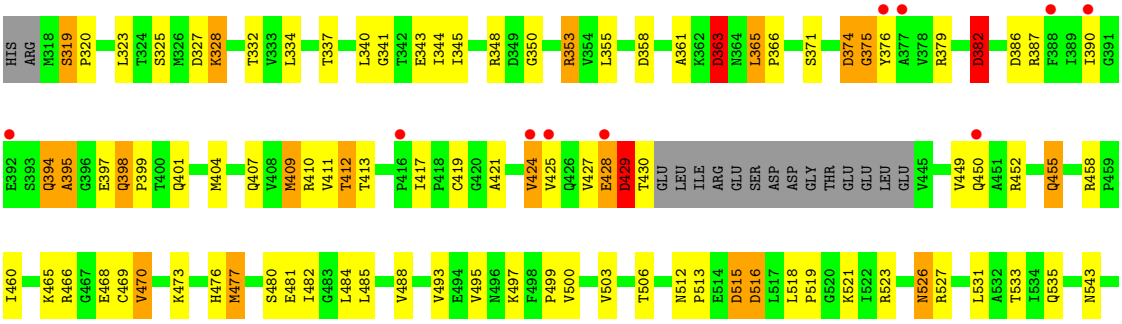
• Molecule 1: Gephyrin

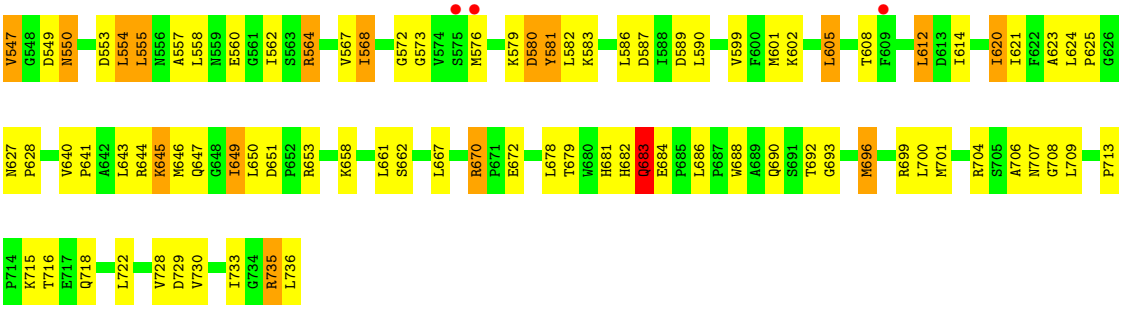
Chain A:



• Molecule 1: Gephyrin

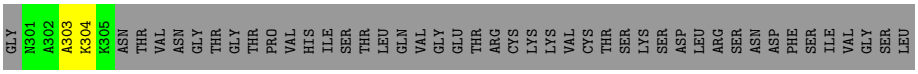
Chain B:





- Molecule 2: 49-mer fragment of Glycine receptor beta chain

Chain P: 6% • 90%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	161.55Å 161.55Å 126.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.25 80.77 – 3.25	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-3.25) 96.8 (80.77-3.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 3.26Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.243 , 0.303 0.220 , 0.277	Depositor DCC
R_{free} test set	1446 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	93.3	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 70.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.073 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6243	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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	0.45	0/3176	0.82	16/4321 (0.4%)
1	B	0.45	0/3124	0.80	11/4250 (0.3%)
2	P	0.51	0/21	0.69	0/26
All	All	0.45	0/6321	0.81	27/8597 (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	1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	553	ASP	CB-CG-OD2	7.71	125.24	118.30
1	B	580	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	374	ASP	CB-CG-OD2	6.27	123.94	118.30
1	B	651	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	549	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	358	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	363	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	552	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	651	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	463	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	358	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	429	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	327	ASP	CB-CG-OD2	5.63	123.37	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	566	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	349	ASP	CB-CG-OD2	5.57	123.32	118.30
1	B	363	ASP	CB-CG-OD2	5.52	123.26	118.30
1	B	382	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	549	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	437	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	613	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	386	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	515	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	386	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	515	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	664	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	587	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	668	ASP	CB-CG-OD2	5.05	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	684	GLU	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	3117	0	3127	110	0
1	B	3064	0	3089	95	0
2	P	22	0	12	0	0
3	A	20	0	0	1	0
3	B	20	0	0	0	0
All	All	6243	0	6228	199	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 16.

All (199) 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:612:LEU:HD13	1:B:614:ILE:HD11	1.13	1.11
1:B:531:LEU:O	1:B:535:GLN:HG3	1.63	0.98
1:B:599:VAL:HG22	1:B:601:MET:HG2	1.51	0.93
1:A:380:ALA:H	1:A:422:ASP:HB2	1.32	0.93
1:B:503:VAL:HB	1:B:531:LEU:HD21	1.49	0.90
1:B:562:ILE:HG13	1:B:568:ILE:HD11	1.59	0.85
1:A:398:GLN:HB2	1:A:399:PRO:HD2	1.59	0.83
1:A:452:ARG:HD2	1:A:455:GLN:HG3	1.60	0.82
1:A:506:THR:OG1	1:A:572:GLY:HA3	1.81	0.80
1:A:391:GLY:O	1:A:409:MET:HG3	1.83	0.76
1:B:513:PRO:HA	1:B:523:ARG:HD3	1.67	0.76
1:A:535:GLN:HE21	1:A:541:THR:HG21	1.51	0.75
1:A:452:ARG:HG3	1:A:455:GLN:HE21	1.53	0.73
1:A:345:ILE:HG12	1:A:495:VAL:HG21	1.69	0.73
1:A:348:ARG:NH2	3:A:8:SO4:O2	2.21	0.72
1:B:599:VAL:CG2	1:B:601:MET:HG2	2.20	0.70
1:B:667:LEU:HD11	1:B:722:LEU:HG	1.71	0.70
1:A:383:GLY:O	1:A:387:ARG:NH2	2.24	0.70
1:A:378:VAL:HG22	1:A:408:VAL:HG12	1.74	0.69
1:A:537:HIS:HE1	1:B:735:ARG:HH21	1.41	0.69
1:A:535:GLN:NE2	1:A:541:THR:HG21	2.08	0.69
1:A:513:PRO:HA	1:A:523:ARG:HD3	1.74	0.69
1:A:488:VAL:HG12	1:A:490:VAL:HG23	1.75	0.68
1:A:398:GLN:HG2	1:A:399:PRO:O	1.93	0.68
1:B:568:ILE:HD12	1:B:621:ILE:HG12	1.74	0.68
1:A:325:SER:HB2	1:A:328:LYS:HB2	1.76	0.67
1:B:363:ASP:HA	1:B:466:ARG:HG3	1.77	0.67
1:B:319:SER:CB	1:B:320:PRO:HD2	2.24	0.67
1:B:518:LEU:HB3	1:B:519:PRO:HD2	1.77	0.66
1:B:681:HIS:O	1:B:683:GLN:N	2.28	0.66
1:B:506:THR:HA	1:B:547:VAL:O	1.98	0.64
1:B:526:ASN:ND2	1:B:526:ASN:H	1.96	0.64
1:B:678:LEU:HB2	1:B:707:ASN:HD22	1.62	0.63
1:B:470:VAL:HG21	1:B:488:VAL:HG21	1.79	0.63
1:A:398:GLN:HB2	1:A:399:PRO:CD	2.29	0.63
1:B:550:ASN:O	1:B:554:LEU:HB2	1.99	0.62
1:B:608:THR:HB	1:B:623:ALA:HB3	1.81	0.62
1:B:337:THR:O	1:B:645:LYS:NZ	2.33	0.62
1:A:709:LEU:HD22	1:A:733:ILE:HG21	1.82	0.61
1:A:452:ARG:O	1:A:455:GLN:HB2	2.00	0.61
1:B:708:GLY:HA2	1:B:733:ILE:HG12	1.82	0.61
1:B:681:HIS:HD2	1:B:688:TRP:CD1	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LYS:HD3	1:A:426:GLN:HE21	1.66	0.60
1:B:374:ASP:HB3	1:B:412:THR:HA	1.83	0.60
1:A:503:VAL:HG22	1:A:569:ILE:HB	1.82	0.60
1:A:537:HIS:CE1	1:B:735:ARG:HH21	2.19	0.60
1:A:337:THR:HG23	1:A:620:ILE:HD12	1.83	0.59
1:B:375:GLY:H	1:B:411:VAL:HG23	1.67	0.59
1:A:369:PRO:HB2	1:A:417:ILE:HB	1.85	0.59
1:A:424:VAL:HG13	1:A:456:ASP:HB2	1.84	0.58
1:A:526:ASN:OD1	1:A:628:PRO:HA	2.03	0.58
1:A:440:THR:HB	1:A:441:GLU:HG2	1.86	0.58
1:A:640:VAL:HB	1:A:641:PRO:HD3	1.86	0.58
1:B:527:ARG:HH11	1:B:543:ASN:HD21	1.52	0.58
1:B:345:ILE:HG12	1:B:495:VAL:HG21	1.87	0.57
1:B:567:VAL:HG13	1:B:620:ILE:HG22	1.86	0.57
1:A:380:ALA:N	1:A:422:ASP:HB2	2.13	0.57
1:A:568:ILE:HB	1:A:621:ILE:HG23	1.87	0.57
1:B:348:ARG:HH11	1:B:348:ARG:HG3	1.69	0.57
1:A:438:ASP:HB3	1:A:440:THR:OG1	2.05	0.57
1:B:328:LYS:O	1:B:332:THR:OG1	2.17	0.57
1:A:379:ARG:HD2	1:A:405:PRO:HA	1.86	0.56
1:B:401:GLN:HB2	1:B:409:MET:CE	2.36	0.56
1:A:709:LEU:HD22	1:A:733:ILE:CG2	2.35	0.56
1:B:337:THR:HG23	1:B:620:ILE:HD12	1.86	0.56
1:B:506:THR:OG1	1:B:572:GLY:HA3	2.04	0.56
1:A:359:VAL:HG13	1:A:490:VAL:HG21	1.86	0.56
1:A:569:ILE:HD11	1:A:639:VAL:HG11	1.88	0.56
1:A:708:GLY:HA2	1:A:733:ILE:HG12	1.88	0.56
1:A:433:ILE:HD11	1:A:446:ARG:HB2	1.88	0.55
1:B:564:ARG:HG2	1:B:564:ARG:HH11	1.71	0.55
1:A:716:THR:HG22	1:A:717:GLU:H	1.71	0.55
1:B:564:ARG:HG2	1:B:564:ARG:NH1	2.20	0.55
1:A:602:LYS:HB3	1:A:672:GLU:HG2	1.87	0.55
1:A:684:GLU:HB3	1:A:685:PRO:CD	2.37	0.55
1:A:500:VAL:O	1:A:565:ALA:HB1	2.07	0.55
1:B:361:ALA:HA	1:B:488:VAL:HG13	1.88	0.55
1:A:608:THR:HB	1:A:623:ALA:HB3	1.88	0.54
1:A:333:VAL:HA	1:A:609:PHE:CE2	2.42	0.54
1:A:426:GLN:HG3	1:A:428:GLU:OE1	2.07	0.54
1:A:333:VAL:O	1:A:337:THR:OG1	2.24	0.54
1:A:542:ILE:HD13	1:A:564:ARG:HB3	1.90	0.53
1:A:345:ILE:HG12	1:A:495:VAL:CG2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ASN:HB3	1:A:514:GLU:OE1	2.09	0.53
1:A:340:LEU:HD11	1:A:499:PRO:HB3	1.91	0.53
1:A:504:MET:HB3	1:A:544:LEU:HB2	1.90	0.53
1:A:535:GLN:HE21	1:A:541:THR:CG2	2.20	0.52
1:B:476:HIS:CE1	1:B:649:ILE:HD11	2.44	0.52
1:B:404:MET:H	1:B:407:GLN:HE21	1.56	0.52
1:A:379:ARG:HA	1:A:422:ASP:H	1.75	0.52
1:B:605:LEU:HD12	1:B:670:ARG:HE	1.75	0.51
1:B:678:LEU:HB2	1:B:707:ASN:ND2	2.24	0.51
1:A:506:THR:HA	1:A:547:VAL:O	2.10	0.51
1:B:481:GLU:OE1	1:B:481:GLU:N	2.43	0.51
1:B:624:LEU:HB3	1:B:625:PRO:HD2	1.90	0.51
1:B:345:ILE:HG12	1:B:495:VAL:CG2	2.41	0.51
1:A:375:GLY:HA2	1:A:427:VAL:HG12	1.92	0.51
1:B:343:GLU:HB2	1:B:497:LYS:HG2	1.93	0.51
1:B:401:GLN:HB2	1:B:409:MET:HE2	1.91	0.51
1:B:427:VAL:HG13	1:B:428:GLU:H	1.76	0.51
1:A:390:ILE:HD11	1:A:407:GLN:NE2	2.26	0.51
1:A:470:VAL:HG21	1:A:488:VAL:HG21	1.93	0.51
1:B:554:LEU:HD11	1:B:582:LEU:HD12	1.92	0.50
1:B:340:LEU:HD11	1:B:499:PRO:HB3	1.93	0.50
1:A:423:ALA:HA	1:A:457:ILE:CD1	2.42	0.50
1:A:684:GLU:HB3	1:A:685:PRO:HD3	1.93	0.49
1:B:612:LEU:CD1	1:B:614:ILE:HD11	2.08	0.49
1:A:373:LYS:HD3	1:A:426:GLN:NE2	2.27	0.49
1:A:602:LYS:O	1:A:672:GLU:HA	2.13	0.49
1:A:461:GLY:HA2	1:A:464:ILE:O	2.12	0.48
1:B:348:ARG:HG3	1:B:348:ARG:NH1	2.27	0.48
1:B:355:LEU:HG	1:B:477:MET:SD	2.54	0.48
1:A:398:GLN:CB	1:A:399:PRO:HD2	2.37	0.48
1:B:526:ASN:H	1:B:526:ASN:HD22	1.62	0.48
1:A:432:LEU:HD21	1:A:442:GLU:HB3	1.95	0.48
1:B:658:LYS:NZ	1:B:729:ASP:OD1	2.44	0.48
1:A:704:ARG:NH1	1:B:644:ARG:HH12	2.11	0.48
1:B:424:VAL:HG12	1:B:455:GLN:O	2.13	0.48
1:B:547:VAL:HG11	1:B:557:ALA:HB2	1.96	0.48
1:B:560:GLU:HG3	1:B:564:ARG:HD3	1.96	0.48
1:B:341:GLY:O	1:B:497:LYS:HG3	2.14	0.47
1:B:602:LYS:O	1:B:672:GLU:HA	2.15	0.47
1:B:580:ASP:O	1:B:581:TYR:C	2.52	0.47
1:A:716:THR:HG22	1:A:717:GLU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:ARG:O	1:B:531:LEU:HG	2.15	0.47
1:A:463:ASP:OD2	1:B:696:MET:HB3	2.15	0.47
1:B:379:ARG:HB2	1:B:382:ASP:HB2	1.96	0.47
1:A:347:TYR:O	1:A:482:ILE:HD13	2.15	0.47
1:A:533:THR:HG21	1:A:635:CYS:SG	2.55	0.46
1:B:564:ARG:HH11	1:B:564:ARG:CG	2.28	0.46
1:A:363:ASP:OD2	1:A:363:ASP:N	2.49	0.46
1:A:359:VAL:CG1	1:A:490:VAL:HG21	2.46	0.46
1:B:374:ASP:CB	1:B:412:THR:HA	2.45	0.46
1:B:394:GLN:O	1:B:395:ALA:C	2.53	0.46
1:B:319:SER:CB	1:B:320:PRO:CD	2.94	0.46
1:A:567:VAL:HG13	1:A:620:ILE:HG22	1.98	0.46
1:A:704:ARG:HH12	1:B:644:ARG:HH12	1.62	0.46
1:B:602:LYS:HB3	1:B:672:GLU:HG2	1.97	0.46
1:A:639:VAL:O	1:A:643:LEU:HG	2.15	0.45
1:A:667:LEU:HB3	1:A:715:LYS:HB3	1.97	0.45
1:A:321:PHE:HE1	1:A:583:LYS:HG3	1.82	0.45
1:A:629:VAL:O	1:A:633:VAL:HG23	2.16	0.45
1:A:512:ASN:O	1:A:514:GLU:N	2.50	0.45
1:B:417:ILE:HG23	1:B:421:ALA:HB3	1.98	0.45
1:A:707:ASN:OD1	1:A:736:LEU:HA	2.17	0.45
1:A:562:ILE:HG23	1:A:619:LYS:HD2	1.99	0.45
1:B:516:ASP:N	1:B:516:ASP:OD1	2.50	0.44
1:A:341:GLY:O	1:A:497:LYS:HG2	2.17	0.44
1:A:395:ALA:HA	1:A:415:ALA:HA	1.99	0.44
1:B:627:ASN:HA	1:B:628:PRO:HD3	1.81	0.44
1:A:337:THR:CG2	1:A:338:PRO:HD2	2.47	0.44
1:A:398:GLN:HB3	1:B:519:PRO:HB2	1.99	0.44
1:B:643:LEU:HD23	1:B:646:MET:HE3	2.00	0.44
1:A:423:ALA:HA	1:A:457:ILE:HD11	2.00	0.44
1:A:569:ILE:HD11	1:A:639:VAL:CG1	2.47	0.44
1:A:458:ARG:HA	1:A:459:PRO:HD3	1.82	0.44
1:A:321:PHE:CE1	1:A:583:LYS:HG3	2.53	0.43
1:B:398:GLN:HA	1:B:399:PRO:HD3	1.90	0.43
1:A:534:ILE:C	1:A:534:ILE:HD12	2.38	0.43
1:A:372:VAL:HG12	1:A:456:ASP:HB3	1.99	0.43
1:A:382:ASP:HB3	1:A:387:ARG:NH1	2.33	0.43
1:B:427:VAL:C	1:B:429:ASP:H	2.21	0.43
1:A:627:ASN:HA	1:A:628:PRO:HD3	1.89	0.43
1:A:673:TYR:HA	1:A:710:LEU:O	2.18	0.43
1:B:558:LEU:O	1:B:562:ILE:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:667:LEU:HD21	1:B:713:PRO:HG2	2.00	0.43
1:A:661:LEU:HD22	1:A:663:CYS:O	2.19	0.43
1:B:693:GLY:HA2	1:B:699:ARG:HB2	2.01	0.43
1:B:350:GLY:O	1:B:353:ARG:HB2	2.18	0.42
1:B:485:LEU:HD23	1:B:485:LEU:HA	1.82	0.42
1:A:506:THR:HG1	1:A:572:GLY:HA3	1.83	0.42
1:A:704:ARG:HD2	1:A:704:ARG:HA	1.86	0.42
1:B:640:VAL:HB	1:B:641:PRO:HD3	2.01	0.42
1:B:667:LEU:HD23	1:B:713:PRO:O	2.19	0.42
1:B:374:ASP:HB3	1:B:413:THR:N	2.34	0.42
1:A:404:MET:CB	1:A:405:PRO:HD2	2.49	0.41
1:B:512:ASN:HB2	1:B:515:ASP:OD2	2.20	0.41
1:B:586:LEU:HA	1:B:590:LEU:HB2	2.02	0.41
1:A:400:THR:HB	1:A:401:GLN:OE1	2.20	0.41
1:A:403:VAL:HG13	1:A:407:GLN:HB2	2.02	0.41
1:A:340:LEU:HD13	1:A:497:LYS:O	2.21	0.41
1:A:398:GLN:CB	1:A:399:PRO:CD	2.93	0.41
1:A:426:GLN:HE21	1:A:426:GLN:HB3	1.61	0.41
1:A:328:LYS:O	1:A:331:ILE:HG22	2.21	0.41
1:A:334:LEU:HD23	1:A:334:LEU:HA	1.88	0.41
1:B:484:LEU:HA	1:B:484:LEU:HD23	1.77	0.41
1:B:365:LEU:HA	1:B:366:PRO:HA	1.91	0.41
1:B:401:GLN:HB2	1:B:409:MET:HE1	2.01	0.41
1:A:351:MET:SD	1:A:479:PRO:HD3	2.61	0.41
1:A:377:ALA:C	1:A:378:VAL:HG23	2.41	0.41
1:B:555:LEU:CD1	1:B:589:ASP:HB3	2.51	0.41
1:B:707:ASN:OD1	1:B:736:LEU:HA	2.20	0.41
1:B:374:ASP:HB3	1:B:412:THR:CA	2.51	0.41
1:A:510:LEU:HB2	1:A:546:ILE:HG21	2.03	0.40
1:B:376:TYR:HB2	1:B:425:VAL:HG22	2.02	0.40
1:B:678:LEU:HD21	1:B:730:VAL:HG11	2.03	0.40
1:A:734:GLY:O	1:A:736:LEU:N	2.54	0.40
1:A:387:ARG:HA	1:A:387:ARG:HD3	1.86	0.40
1:A:458:ARG:HE	1:A:462:HIS:CE1	2.40	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	406/421 (96%)	367 (90%)	28 (7%)	11 (3%)	5 26
1	B	401/421 (95%)	349 (87%)	42 (10%)	10 (2%)	5 28
2	P	3/49 (6%)	1 (33%)	0	2 (67%)	0 0
All	All	810/891 (91%)	717 (88%)	70 (9%)	23 (3%)	5 25

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	440	THR
1	A	682	HIS
1	B	419	CYS
1	B	682	HIS
1	B	696	MET
1	A	433	ILE
1	A	573	GLY
1	A	693	GLY
1	A	701	MET
1	B	395	ALA
1	B	573	GLY
1	B	735	ARG
2	P	303	ALA
1	A	735	ARG
1	B	683	GLN
1	A	398	GLN
1	A	460	ILE
1	B	706	ALA
2	P	304	LYS
1	A	405	PRO
1	B	319	SER
1	B	375	GLY
1	A	685	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	341/358 (95%)	277 (81%)	64 (19%)	1 6
1	B	337/358 (94%)	258 (77%)	79 (23%)	1 3
All	All	678/716 (95%)	535 (79%)	143 (21%)	1 4

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	LEU
1	A	327	ASP
1	A	328	LYS
1	A	331	ILE
1	A	343	GLU
1	A	344	ILE
1	A	353	ARG
1	A	363	ASP
1	A	372	VAL
1	A	397	GLU
1	A	398	GLN
1	A	401	GLN
1	A	404	MET
1	A	419	CYS
1	A	426	GLN
1	A	440	THR
1	A	442	GLU
1	A	452	ARG
1	A	458	ARG
1	A	460	ILE
1	A	465	LYS
1	A	473	LYS
1	A	480	SER
1	A	481	GLU
1	A	492	GLU
1	A	493	VAL
1	A	495	VAL

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Mol	Chain	Res	Type
1	A	508	ASN
1	A	510	LEU
1	A	516	ASP
1	A	525	SER
1	A	528	SER
1	A	529	THR
1	A	533	THR
1	A	541	THR
1	A	546	ILE
1	A	554	LEU
1	A	563	SER
1	A	564	ARG
1	A	570	THR
1	A	574	VAL
1	A	581	TYR
1	A	599	VAL
1	A	600	PHE
1	A	605	LEU
1	A	613	ASP
1	A	614	ILE
1	A	615	ASP
1	A	620	ILE
1	A	621	ILE
1	A	647	GLN
1	A	649	ILE
1	A	662	SER
1	A	668	ASP
1	A	670	ARG
1	A	675	ARG
1	A	679	THR
1	A	682	HIS
1	A	690	GLN
1	A	701	MET
1	A	704	ARG
1	A	715	LYS
1	A	721	GLU
1	A	728	VAL
1	B	323	LEU
1	B	325	SER
1	B	328	LYS
1	B	334	LEU
1	B	344	ILE

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Mol	Chain	Res	Type
1	B	353	ARG
1	B	363	ASP
1	B	365	LEU
1	B	371	SER
1	B	374	ASP
1	B	382	ASP
1	B	387	ARG
1	B	390	ILE
1	B	394	GLN
1	B	397	GLU
1	B	398	GLN
1	B	409	MET
1	B	410	ARG
1	B	412	THR
1	B	424	VAL
1	B	428	GLU
1	B	429	ASP
1	B	430	THR
1	B	449	VAL
1	B	450	GLN
1	B	452	ARG
1	B	455	GLN
1	B	458	ARG
1	B	460	ILE
1	B	465	LYS
1	B	468	GLU
1	B	469	CYS
1	B	470	VAL
1	B	473	LYS
1	B	477	MET
1	B	480	SER
1	B	482	ILE
1	B	493	VAL
1	B	500	VAL
1	B	516	ASP
1	B	521	LYS
1	B	526	ASN
1	B	533	THR
1	B	547	VAL
1	B	550	ASN
1	B	553	ASP
1	B	554	LEU

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Mol	Chain	Res	Type
1	B	555	LEU
1	B	564	ARG
1	B	568	ILE
1	B	576	MET
1	B	579	LYS
1	B	581	TYR
1	B	583	LYS
1	B	605	LEU
1	B	612	LEU
1	B	620	ILE
1	B	645	LYS
1	B	647	GLN
1	B	649	ILE
1	B	650	LEU
1	B	653	ARG
1	B	661	LEU
1	B	662	SER
1	B	670	ARG
1	B	679	THR
1	B	683	GLN
1	B	684	GLU
1	B	686	LEU
1	B	690	GLN
1	B	692	THR
1	B	700	LEU
1	B	701	MET
1	B	704	ARG
1	B	709	LEU
1	B	715	LYS
1	B	716	THR
1	B	718	GLN
1	B	728	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	GLN
1	A	426	GLN
1	A	455	GLN
1	A	535	GLN
1	A	537	HIS
1	A	690	GLN

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Mol	Chain	Res	Type
1	B	394	GLN
1	B	407	GLN
1	B	526	ASN
1	B	535	GLN
1	B	593	GLN
1	B	681	HIS

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)

8 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	B	1	-	4,4,4	0.21	0	6,6,6	0.27	0
3	SO4	A	8	-	4,4,4	0.24	0	6,6,6	0.22	0
3	SO4	B	4	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	A	7	-	4,4,4	0.23	0	6,6,6	0.19	0
3	SO4	A	2	-	4,4,4	0.25	0	6,6,6	0.15	0
3	SO4	B	3	-	4,4,4	0.27	0	6,6,6	0.15	0
3	SO4	B	5	-	4,4,4	0.25	0	6,6,6	0.18	0
3	SO4	A	6	-	4,4,4	0.29	0	6,6,6	0.17	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	8	SO4	1	0

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 (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	412/421 (97%)	0.26	6 (1%) 73 71	13, 38, 75, 93	0
1	B	405/421 (96%)	0.32	13 (3%) 47 45	13, 45, 90, 105	0
2	P	5/49 (10%)	0.17	0 100 100	78, 79, 80, 81	0
All	All	822/891 (92%)	0.29	19 (2%) 60 58	13, 41, 84, 105	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	390	ILE	3.6
1	B	424	VAL	3.4
1	B	388	PHE	2.9
1	B	425	VAL	2.8
1	B	428	GLU	2.6
1	B	609	PHE	2.6
1	B	416	PRO	2.5
1	A	442	GLU	2.5
1	B	392	GLU	2.5
1	B	576	MET	2.5
1	B	575	SER	2.4
1	A	730	VAL	2.4
1	A	678	LEU	2.3
1	B	376	TYR	2.2
1	A	318	MET	2.2
1	A	319	SER	2.2
1	B	377	ALA	2.1
1	A	609	PHE	2.1
1	B	450	GLN	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, 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	A	7	5/5	0.71	0.33	74,74,74,75	5
3	SO4	A	2	5/5	0.74	0.51	82,82,82,82	5
3	SO4	A	6	5/5	0.89	0.18	64,64,65,65	5
3	SO4	A	8	5/5	0.92	0.17	46,46,46,46	5
3	SO4	B	4	5/5	0.92	0.22	60,60,61,61	5
3	SO4	B	5	5/5	0.93	0.22	66,67,67,67	5
3	SO4	B	1	5/5	0.94	0.19	55,56,56,56	5
3	SO4	B	3	5/5	0.96	0.20	50,50,51,51	5

6.5 Other polymers (i)

There are no such residues in this entry.