



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:33 AM UTC

PDB ID : 7ESG / pdb_00007esg
Title : Crystal structure of Haloarcula marismortui CheB with Glutathione S-transferase expression tag
Authors : Chen, K.L.; Yang, C.S.
Deposited on : 2021-05-10
Resolution : 2.53 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

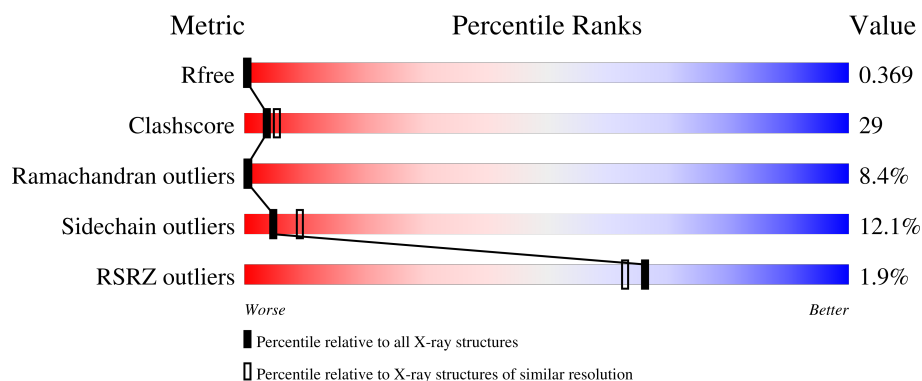
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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 $\leq 5\%$. 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	598	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4553 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 Glutathione S-transferase,Protein-glutamate methylesterase/protein-glutamine glutaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	0	0	0
			4514	2822	767	895	30			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	SER	-	linker	UNP P08515
A	220	ASP	-	linker	UNP P08515
A	221	LEU	-	linker	UNP P08515
A	222	VAL	-	linker	UNP P08515
A	223	PRO	-	linker	UNP P08515
A	224	ARG	-	linker	UNP P08515
A	225	GLY	-	linker	UNP P08515
A	226	SER	-	linker	UNP P08515
A	227	PRO	-	linker	UNP P08515
A	228	GLU	-	linker	UNP P08515
A	229	PHE	-	linker	UNP P08515

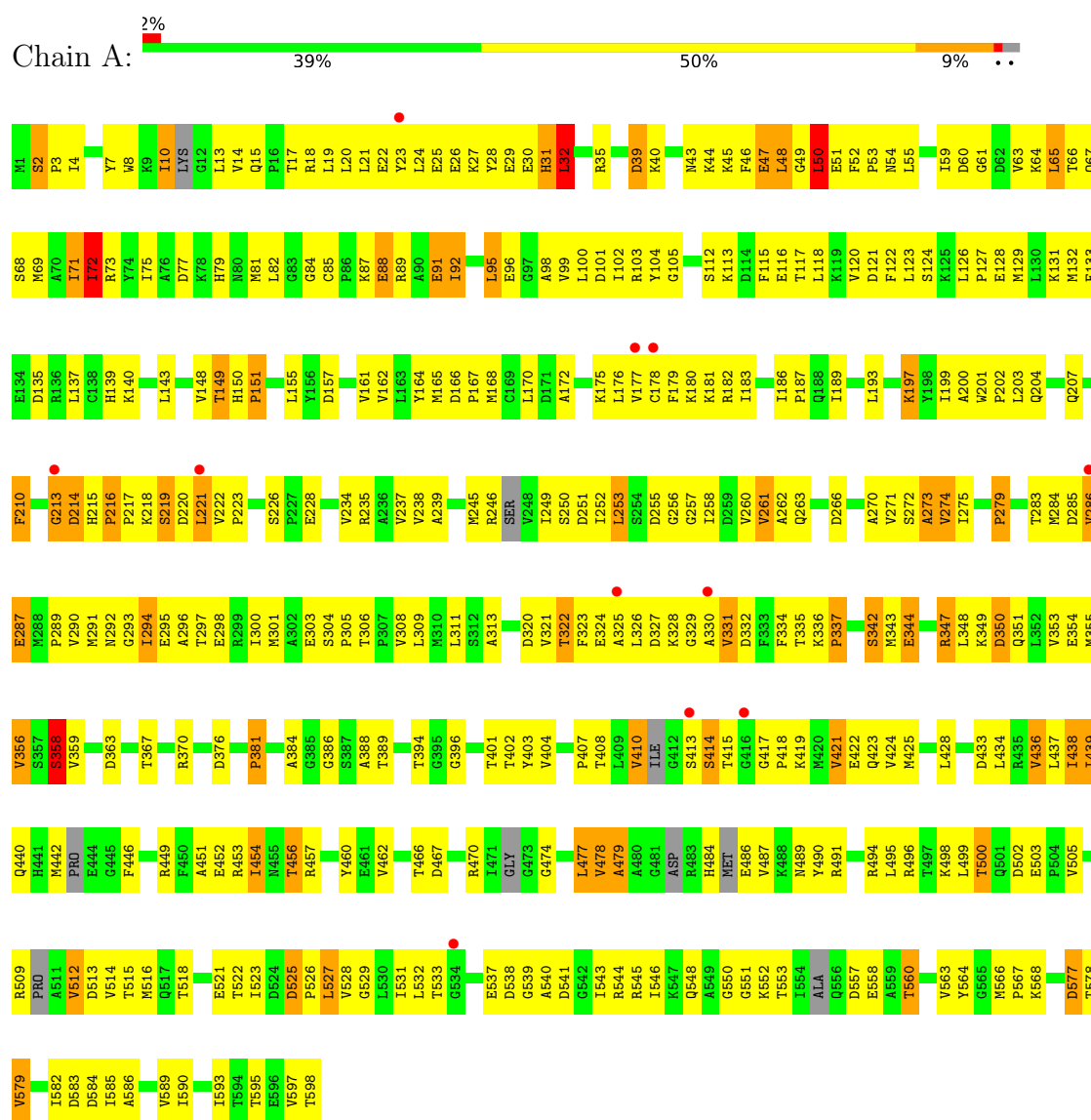
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	39	Total	O	0	0
			39	39		

3 Residue-property plots

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: Glutathione S-transferase,Protein-glutamate methylesterase/protein-glutamine glutaminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.06Å 93.91Å 93.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.86 – 2.53 23.86 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.5 (23.86-2.53) 98.9 (23.86-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	120.76 (at 2.53Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.349 , 0.372 0.346 , 0.369	Depositor DCC
R_{free} test set	1753 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 113.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.318 for -h,l,k	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	4553	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

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	0.15	0/4585	0.46	0/6191

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 [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	4514	0	4445	260	0
2	A	39	0	0	11	0
All	All	4553	0	4445	260	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 29.

All (260) 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:295:GLU:OE1	2:A:601:HOH:O	1.85	0.94
1:A:140:LYS:HA	1:A:143:LEU:HB2	1.51	0.92
1:A:161:VAL:O	2:A:602:HOH:O	1.91	0.89
1:A:137:LEU:HB3	1:A:151:PRO:HB3	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ARG:H	1:A:249:ILE:HB	1.41	0.85
1:A:586:ALA:HA	1:A:589:VAL:HG12	1.57	0.85
1:A:172:ALA:HA	1:A:175:LYS:HB3	1.61	0.83
1:A:71:ILE:HA	1:A:210:PHE:HB3	1.61	0.82
1:A:53:PRO:HB3	1:A:199:ILE:HD11	1.62	0.81
1:A:178:CYS:SG	2:A:618:HOH:O	2.38	0.81
1:A:238:VAL:HG13	1:A:246:ARG:HB3	1.61	0.80
1:A:126:LEU:HD12	1:A:129:MET:HG2	1.64	0.80
1:A:521:GLU:O	2:A:603:HOH:O	2.01	0.79
1:A:53:PRO:HG2	1:A:222:VAL:HG22	1.64	0.79
1:A:72:ILE:HG21	1:A:216:PRO:HD2	1.65	0.79
1:A:101:ASP:HA	1:A:104:TYR:HB3	1.64	0.78
1:A:327:ASP:OD1	2:A:604:HOH:O	2.01	0.78
1:A:148:VAL:O	1:A:150:HIS:N	2.16	0.77
1:A:531:ILE:HD11	1:A:539:GLY:HA3	1.67	0.77
1:A:298:GLU:HA	1:A:301:MET:HB2	1.67	0.76
1:A:168:MET:HA	1:A:172:ALA:HB3	1.69	0.75
1:A:35:ARG:HB3	1:A:39:ASP:HB2	1.69	0.75
1:A:347:ARG:NH2	2:A:607:HOH:O	2.16	0.72
1:A:29:GLU:HA	1:A:32:LEU:HD13	1.71	0.71
1:A:98:ALA:O	1:A:102:ILE:N	2.23	0.71
1:A:2:SER:H	1:A:3:PRO:HD2	1.56	0.71
1:A:252:ILE:HG23	1:A:253:LEU:HG	1.72	0.71
1:A:246:ARG:HH22	1:A:253:LEU:HD21	1.56	0.70
1:A:167:PRO:O	1:A:172:ALA:N	2.20	0.70
1:A:531:ILE:HD13	1:A:566:MET:HE3	1.74	0.70
1:A:337:PRO:HG2	1:A:348:LEU:HD21	1.74	0.70
1:A:417:GLY:HA2	1:A:421:VAL:HB	1.73	0.69
1:A:31:HIS:O	1:A:43:ASN:ND2	2.26	0.69
1:A:135:ASP:O	1:A:139:HIS:NE2	2.25	0.69
1:A:320:ASP:O	1:A:324:GLU:N	2.26	0.69
1:A:95:LEU:HD23	1:A:98:ALA:HB3	1.74	0.68
1:A:410:VAL:HA	1:A:437:LEU:H	1.57	0.68
1:A:200:ALA:HA	1:A:203:LEU:HB3	1.76	0.68
1:A:73:ARG:HD3	1:A:217:PRO:HG3	1.76	0.67
1:A:424:VAL:HG22	1:A:585:ILE:HG13	1.76	0.67
1:A:54:ASN:OD1	2:A:605:HOH:O	2.12	0.67
1:A:186:ILE:HA	1:A:189:ILE:HG12	1.75	0.66
1:A:578:THR:HG22	1:A:579:VAL:H	1.60	0.66
1:A:87:LYS:HB3	1:A:509:ARG:HE	1.60	0.66
1:A:44:LYS:O	1:A:46:PHE:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:HD23	1:A:199:ILE:HD13	1.79	0.64
1:A:123:LEU:HA	1:A:126:LEU:HB2	1.78	0.64
1:A:355:MET:O	1:A:359:VAL:N	2.31	0.63
1:A:286:VAL:HG23	1:A:321:VAL:HG11	1.80	0.63
1:A:414:SER:OG	1:A:415:THR:N	2.29	0.62
1:A:283:THR:HG22	1:A:311:LEU:HD21	1.81	0.62
1:A:79:HIS:HD2	1:A:537:GLU:H	1.48	0.62
1:A:297:THR:O	1:A:301:MET:N	2.32	0.61
1:A:24:LEU:HD11	1:A:218:LYS:HE3	1.82	0.61
1:A:237:VAL:HG23	1:A:279:PRO:HG2	1.82	0.61
1:A:518:THR:O	1:A:522:THR:OG1	2.18	0.61
1:A:237:VAL:HG21	1:A:274:VAL:HA	1.82	0.61
1:A:238:VAL:HB	1:A:263:GLN:HA	1.83	0.61
1:A:99:VAL:HA	1:A:102:ILE:HB	1.83	0.61
1:A:10:ILE:HG23	1:A:13:LEU:HB3	1.84	0.60
1:A:545:ARG:HA	1:A:548:GLN:HB2	1.84	0.60
1:A:72:ILE:HD13	1:A:216:PRO:HG2	1.84	0.60
1:A:543:ILE:HG22	1:A:546:ILE:HD12	1.84	0.60
1:A:15:GLN:O	1:A:19:LEU:HB2	2.01	0.60
1:A:8:TRP:HD1	1:A:234:VAL:HG22	1.67	0.59
1:A:442:MET:HB3	1:A:446:PHE:HD2	1.68	0.59
1:A:200:ALA:O	1:A:204:GLN:N	2.31	0.58
1:A:546:ILE:HG22	1:A:551:GLY:HA3	1.86	0.58
1:A:408:THR:HB	1:A:528:VAL:HG12	1.86	0.58
1:A:437:LEU:HD12	1:A:477:LEU:HD22	1.86	0.58
1:A:466:THR:OG1	1:A:467:ASP:N	2.37	0.57
1:A:199:ILE:HG13	1:A:200:ALA:N	2.20	0.57
1:A:419:LYS:NZ	1:A:423:GLN:OE1	2.37	0.57
1:A:454:ILE:HG22	1:A:460:TYR:HE1	1.70	0.57
1:A:528:VAL:HG23	1:A:552:LYS:HB2	1.87	0.56
1:A:113:LYS:HA	1:A:116:GLU:HB2	1.87	0.56
1:A:394:THR:HG22	1:A:396:GLY:H	1.70	0.56
1:A:179:PHE:HA	1:A:182:ARG:HB2	1.87	0.55
1:A:239:ALA:HB3	1:A:284:MET:HA	1.86	0.55
1:A:67:GLN:O	1:A:71:ILE:HG13	2.06	0.55
1:A:577:ASP:OD1	1:A:577:ASP:N	2.39	0.55
1:A:424:VAL:HG21	1:A:532:LEU:HD11	1.89	0.55
1:A:72:ILE:CG2	1:A:216:PRO:HD2	2.34	0.54
1:A:73:ARG:NE	1:A:77:ASP:OD2	2.40	0.54
1:A:344:GLU:O	1:A:348:LEU:N	2.36	0.54
1:A:53:PRO:HD2	1:A:222:VAL:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:O	1:A:129:MET:HG3	2.07	0.54
1:A:478:VAL:HG12	1:A:479:ALA:H	1.73	0.54
1:A:20:LEU:O	1:A:24:LEU:HD12	2.08	0.54
1:A:332:ASP:OD2	1:A:415:THR:OG1	2.25	0.54
1:A:180:LYS:O	1:A:180:LYS:NZ	2.33	0.53
1:A:286:VAL:HG13	1:A:287:GLU:H	1.72	0.53
1:A:255:ASP:OD1	2:A:608:HOH:O	2.17	0.53
1:A:477:LEU:N	2:A:611:HOH:O	2.40	0.52
1:A:452:GLU:O	1:A:456:THR:OG1	2.27	0.52
1:A:50:LEU:HB3	1:A:219:SER:HB3	1.91	0.52
1:A:470:ARG:HD2	1:A:496:ARG:HG2	1.90	0.52
1:A:558:GLU:HA	1:A:564:TYR:CZ	2.44	0.52
1:A:88:GLU:HG3	1:A:509:ARG:H	1.72	0.52
1:A:418:PRO:O	1:A:422:GLU:HG3	2.09	0.52
1:A:101:ASP:HA	1:A:104:TYR:CB	2.37	0.52
1:A:4:ILE:HA	1:A:7:TYR:HB2	1.92	0.52
1:A:22:GLU:O	1:A:26:GLU:HB2	2.10	0.52
1:A:193:LEU:HD23	1:A:199:ILE:CD1	2.40	0.51
1:A:214:ASP:OD1	1:A:215:HIS:N	2.42	0.51
1:A:63:VAL:O	1:A:66:THR:HG22	2.11	0.51
1:A:222:VAL:HG11	1:A:226:SER:OG	2.10	0.51
1:A:235:ARG:HE	1:A:279:PRO:HA	1.75	0.51
1:A:381:PRO:HG3	1:A:584:ASP:OD1	2.11	0.51
1:A:4:ILE:O	1:A:8:TRP:N	2.41	0.50
1:A:179:PHE:CD1	1:A:182:ARG:HD3	2.46	0.50
1:A:82:LEU:HD22	1:A:350:ASP:HB2	1.92	0.50
1:A:137:LEU:HD13	1:A:151:PRO:HA	1.93	0.50
1:A:91:GLU:C	1:A:92:ILE:HG13	2.36	0.50
1:A:326:LEU:HD12	1:A:327:ASP:N	2.27	0.50
1:A:54:ASN:HB3	1:A:55:LEU:HD12	1.94	0.50
1:A:285:ASP:OD1	1:A:286:VAL:HG12	2.12	0.50
1:A:213:GLY:O	1:A:214:ASP:HB3	2.11	0.50
1:A:525:ASP:HB3	1:A:526:PRO:CD	2.42	0.50
1:A:271:VAL:HG22	1:A:300:ILE:HB	1.94	0.49
1:A:304:SER:O	1:A:304:SER:OG	2.30	0.49
1:A:320:ASP:HB2	1:A:449:ARG:HH11	1.77	0.49
1:A:238:VAL:HG22	1:A:246:ARG:HH11	1.77	0.49
1:A:304:SER:O	1:A:306:THR:N	2.45	0.49
1:A:350:ASP:O	1:A:354:GLU:HB3	2.13	0.49
1:A:293:GLY:HA2	1:A:296:ALA:HB3	1.95	0.49
1:A:541:ASP:HA	1:A:544:ARG:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:VAL:C	1:A:358:SER:H	2.21	0.48
1:A:172:ALA:O	1:A:176:LEU:N	2.42	0.48
1:A:30:GLU:O	1:A:32:LEU:N	2.46	0.48
1:A:193:LEU:HB3	1:A:199:ILE:HD13	1.96	0.48
1:A:294:ILE:HD11	1:A:321:VAL:HG22	1.96	0.48
1:A:453:ARG:HD2	1:A:457:ARG:HD2	1.96	0.48
1:A:514:VAL:O	1:A:518:THR:HG23	2.13	0.48
1:A:258:ILE:HD12	1:A:353:VAL:HB	1.95	0.48
1:A:120:VAL:O	1:A:124:SER:N	2.46	0.48
1:A:486:GLU:N	1:A:500:THR:HG1	2.12	0.48
1:A:59:ILE:O	1:A:61:GLY:N	2.46	0.48
1:A:79:HIS:CD2	1:A:537:GLU:H	2.31	0.48
1:A:85:CYS:SG	1:A:88:GLU:N	2.87	0.48
1:A:235:ARG:HB2	1:A:279:PRO:HA	1.96	0.47
1:A:404:VAL:HG12	1:A:597:VAL:HB	1.96	0.47
1:A:2:SER:N	1:A:3:PRO:HD2	2.28	0.47
1:A:177:VAL:O	1:A:181:LYS:N	2.30	0.47
1:A:75:ILE:HG13	1:A:79:HIS:CG	2.50	0.47
1:A:199:ILE:O	1:A:202:PRO:HD2	2.14	0.47
1:A:593:ILE:HG13	1:A:597:VAL:HG11	1.96	0.46
1:A:356:VAL:HA	1:A:359:VAL:HB	1.98	0.46
1:A:358:SER:O	1:A:563:VAL:HG21	2.16	0.46
1:A:384:ALA:HA	1:A:388:ALA:HB3	1.97	0.46
1:A:91:GLU:O	1:A:92:ILE:HG13	2.16	0.46
1:A:326:LEU:HA	1:A:330:ALA:HB3	1.97	0.46
1:A:148:VAL:HG13	1:A:150:HIS:CD2	2.50	0.46
1:A:428:LEU:HD22	1:A:434:LEU:HD13	1.97	0.46
1:A:148:VAL:C	1:A:150:HIS:N	2.73	0.46
1:A:21:LEU:HA	1:A:24:LEU:HD13	1.97	0.46
1:A:505:VAL:HG21	1:A:514:VAL:HB	1.97	0.46
1:A:69:MET:HB2	1:A:216:PRO:O	2.16	0.46
1:A:326:LEU:HB2	1:A:418:PRO:HB3	1.96	0.46
1:A:63:VAL:O	1:A:67:GLN:HG3	2.16	0.46
1:A:566:MET:HB3	1:A:567:PRO:HD3	1.98	0.46
1:A:403:TYR:HA	1:A:598:THR:HA	1.98	0.45
1:A:410:VAL:O	1:A:436:VAL:HG23	2.15	0.45
1:A:266:ASP:HA	1:A:289:PRO:HG2	1.99	0.45
1:A:334:PHE:CE2	1:A:337:PRO:HD3	2.52	0.45
1:A:424:VAL:HG13	1:A:585:ILE:HB	1.99	0.45
1:A:487:VAL:HG23	1:A:496:ARG:H	1.82	0.45
1:A:47:GLU:O	1:A:49:GLY:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:HG13	1:A:79:HIS:ND1	2.32	0.45
1:A:301:MET:HE2	1:A:329:GLY:HA3	1.99	0.45
1:A:478:VAL:HG12	1:A:479:ALA:N	2.31	0.45
1:A:52:PHE:HD2	1:A:55:LEU:HB2	1.81	0.45
1:A:64:LYS:O	1:A:68:SER:N	2.34	0.45
1:A:161:VAL:HA	1:A:164:TYR:HB3	1.98	0.45
1:A:262:ALA:HB1	1:A:273:ALA:HB1	1.98	0.45
1:A:590:ILE:O	1:A:593:ILE:HG22	2.16	0.45
1:A:523:ILE:HG21	1:A:527:LEU:HD13	1.97	0.45
1:A:65:LEU:HD13	1:A:65:LEU:HA	1.83	0.44
1:A:112:SER:HA	1:A:115:PHE:HD2	1.82	0.44
1:A:292:ASN:OD1	1:A:293:GLY:N	2.51	0.44
1:A:370:ARG:NH2	1:A:560:THR:O	2.50	0.44
1:A:50:LEU:HB2	1:A:51:GLU:H	1.51	0.44
1:A:162:VAL:HA	1:A:165:MET:HE3	1.99	0.44
1:A:557:ASP:OD1	1:A:558:GLU:N	2.51	0.44
1:A:81:MET:HE3	1:A:92:ILE:HG12	1.98	0.44
1:A:177:VAL:HA	1:A:180:LYS:HB3	2.00	0.44
1:A:270:ALA:O	1:A:273:ALA:N	2.51	0.44
1:A:326:LEU:HD13	1:A:418:PRO:O	2.18	0.44
1:A:437:LEU:HD21	1:A:515:THR:HG23	1.99	0.44
1:A:79:HIS:HD2	1:A:537:GLU:N	2.15	0.43
1:A:127:PRO:O	1:A:131:LYS:HB2	2.17	0.43
1:A:525:ASP:HB3	1:A:526:PRO:HD2	2.00	0.43
1:A:532:LEU:HD23	1:A:532:LEU:HA	1.86	0.43
1:A:121:ASP:OD1	1:A:122:PHE:N	2.51	0.43
1:A:126:LEU:HD12	1:A:126:LEU:HA	1.87	0.43
1:A:349:LYS:O	1:A:353:VAL:HG22	2.18	0.43
1:A:538:ASP:C	1:A:540:ALA:H	2.27	0.43
1:A:23:TYR:O	1:A:27:LYS:HB2	2.17	0.43
1:A:197:LYS:HB2	1:A:197:LYS:HE3	1.80	0.43
1:A:126:LEU:N	1:A:127:PRO:HD2	2.34	0.43
1:A:331:VAL:HG13	1:A:332:ASP:H	1.83	0.43
1:A:438:ILE:O	1:A:439:ILE:C	2.62	0.43
1:A:238:VAL:HG23	1:A:260:VAL:HG23	2.00	0.43
1:A:245:MET:SD	1:A:245:MET:N	2.88	0.43
1:A:336:LYS:HA	1:A:337:PRO:HD3	1.84	0.43
1:A:297:THR:OG1	1:A:308:VAL:HG11	2.19	0.43
1:A:404:VAL:HG22	1:A:494:ARG:HH22	1.84	0.43
1:A:133:PHE:HD1	1:A:133:PHE:HA	1.75	0.43
1:A:484:HIS:N	1:A:500:THR:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:HIS:NE2	1:A:537:GLU:HB3	2.34	0.43
1:A:118:LEU:HD22	1:A:178:CYS:HB2	2.00	0.43
1:A:193:LEU:HA	1:A:199:ILE:HG21	2.00	0.43
1:A:24:LEU:HD22	1:A:48:LEU:HD13	2.00	0.43
1:A:166:ASP:HB3	1:A:167:PRO:HD2	2.00	0.43
1:A:182:ARG:O	1:A:186:ILE:HG23	2.19	0.42
1:A:220:ASP:O	1:A:222:VAL:N	2.49	0.42
1:A:148:VAL:HG12	1:A:149:THR:N	2.34	0.42
1:A:386:GLY:HA3	1:A:590:ILE:HG22	2.01	0.42
1:A:421:VAL:HG22	1:A:425:MET:HE2	2.00	0.42
1:A:19:LEU:HD23	2:A:607:HOH:O	2.20	0.42
1:A:275:ILE:HG23	1:A:300:ILE:HD11	2.01	0.42
1:A:287:GLU:O	1:A:287:GLU:HG3	2.20	0.42
1:A:251:ASP:OD1	1:A:251:ASP:N	2.52	0.42
1:A:529:GLY:O	1:A:553:THR:HA	2.20	0.42
1:A:502:ASP:CG	1:A:503:GLU:H	2.28	0.42
1:A:582:ILE:HA	1:A:585:ILE:HD11	2.02	0.42
1:A:313:ALA:N	1:A:336:LYS:HB3	2.35	0.42
1:A:454:ILE:H	1:A:454:ILE:HG13	1.57	0.42
1:A:166:ASP:O	1:A:170:LEU:N	2.51	0.42
1:A:214:ASP:CG	1:A:216:PRO:HD3	2.45	0.42
1:A:234:VAL:O	1:A:258:ILE:HA	2.19	0.42
1:A:326:LEU:HD22	1:A:418:PRO:HA	2.01	0.42
1:A:292:ASN:O	1:A:296:ALA:N	2.52	0.42
1:A:140:LYS:HG2	1:A:143:LEU:HD22	2.02	0.42
1:A:271:VAL:HA	1:A:300:ILE:HD12	2.02	0.42
1:A:347:ARG:HH11	1:A:347:ARG:HB2	1.85	0.42
1:A:407:PRO:HB3	1:A:434:LEU:HA	2.02	0.42
1:A:24:LEU:O	1:A:28:TYR:HB3	2.20	0.41
1:A:425:MET:SD	1:A:425:MET:N	2.94	0.41
1:A:513:ASP:HB2	1:A:538:ASP:HB3	2.01	0.41
1:A:228:GLU:OE1	1:A:228:GLU:N	2.53	0.41
1:A:322:THR:HB	1:A:323:PHE:CD1	2.55	0.41
1:A:394:THR:HG22	1:A:396:GLY:N	2.35	0.41
1:A:486:GLU:O	1:A:498:LYS:HB3	2.20	0.41
1:A:96:GLU:O	1:A:100:LEU:HB2	2.21	0.41
1:A:512:VAL:O	1:A:516:MET:HG3	2.20	0.41
1:A:89:ARG:NH1	1:A:351:GLN:OE1	2.54	0.41
1:A:215:HIS:NE2	2:A:607:HOH:O	2.15	0.41
1:A:235:ARG:HB3	1:A:261:VAL:CG2	2.51	0.41
1:A:342:SER:HB2	1:A:343:MET:H	1.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:SER:O	1:A:440:GLN:HA	2.21	0.41
1:A:564:TYR:O	1:A:568:LYS:HB2	2.21	0.40
1:A:10:ILE:HG21	1:A:221:LEU:HD22	2.02	0.40
1:A:128:GLU:O	1:A:132:MET:HB2	2.21	0.40
1:A:325:ALA:HA	1:A:328:LYS:HB2	2.03	0.40
1:A:410:VAL:CA	1:A:437:LEU:H	2.29	0.40
1:A:451:ALA:HB1	1:A:462:VAL:HG13	2.02	0.40
1:A:491:ARG:HE	1:A:491:ARG:HB3	1.74	0.40
1:A:417:GLY:N	1:A:418:PRO:HD2	2.36	0.40
1:A:495:LEU:HD11	1:A:523:ILE:HB	2.03	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	569/598 (95%)	399 (70%)	122 (21%)	48 (8%)	0 0

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	LYS
1	A	149	THR
1	A	216	PRO
1	A	358	SER
1	A	381	PRO
1	A	478	VAL
1	A	490	TYR
1	A	17	THR
1	A	31	HIS
1	A	32	LEU
1	A	60	ASP

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Mol	Chain	Res	Type
1	A	72	ILE
1	A	261	VAL
1	A	279	PRO
1	A	303	GLU
1	A	337	PRO
1	A	363	ASP
1	A	414	SER
1	A	477	LEU
1	A	71	ILE
1	A	105	GLY
1	A	214	ASP
1	A	219	SER
1	A	223	PRO
1	A	479	ALA
1	A	525	ASP
1	A	48	LEU
1	A	187	PRO
1	A	256	GLY
1	A	273	ALA
1	A	290	VAL
1	A	583	ASP
1	A	91	GLU
1	A	210	PHE
1	A	213	GLY
1	A	221	LEU
1	A	344	GLU
1	A	50	LEU
1	A	151	PRO
1	A	291	MET
1	A	257	GLY
1	A	439	ILE
1	A	474	GLY
1	A	2	SER
1	A	84	GLY
1	A	92	ILE
1	A	305	PRO
1	A	550	GLY

5.3.2 Protein sidechains

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	488/495 (99%)	429 (88%)	59 (12%)	5 9

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	14	VAL
1	A	18	ARG
1	A	25	GLU
1	A	32	LEU
1	A	39	ASP
1	A	40	LYS
1	A	47	GLU
1	A	50	LEU
1	A	65	LEU
1	A	72	ILE
1	A	88	GLU
1	A	95	LEU
1	A	103	ARG
1	A	117	THR
1	A	155	LEU
1	A	157	ASP
1	A	183	ILE
1	A	197	LYS
1	A	201	TRP
1	A	207	GLN
1	A	250	SER
1	A	253	LEU
1	A	272	SER
1	A	274	VAL
1	A	286	VAL
1	A	287	GLU
1	A	294	ILE
1	A	309	LEU
1	A	322	THR
1	A	331	VAL
1	A	335	THR
1	A	342	SER
1	A	347	ARG

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Mol	Chain	Res	Type
1	A	350	ASP
1	A	356	VAL
1	A	358	SER
1	A	367	THR
1	A	376	ASP
1	A	389	THR
1	A	401	THR
1	A	402	THR
1	A	410	VAL
1	A	421	VAL
1	A	433	ASP
1	A	436	VAL
1	A	438	ILE
1	A	454	ILE
1	A	456	THR
1	A	489	ASN
1	A	499	LEU
1	A	500	THR
1	A	512	VAL
1	A	527	LEU
1	A	533	THR
1	A	560	THR
1	A	577	ASP
1	A	579	VAL
1	A	595	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	GLN
1	A	427	ASN
1	A	440	GLN
1	A	463	GLN

5.3.3 RNA ⓘ

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](#)

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](#)

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	589/598 (98%)	0.12	11 (1%) 66 63	23, 27, 31, 35	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	416	GLY	7.6
1	A	178	CYS	4.2
1	A	330	ALA	3.0
1	A	221	LEU	2.7
1	A	23	TYR	2.6
1	A	286	VAL	2.5
1	A	213	GLY	2.4
1	A	177	VAL	2.2
1	A	534	GLY	2.2
1	A	325	ALA	2.1
1	A	413	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.