



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 12:14 AM GMT

PDB ID : 3ANS
Title : Human soluble epoxide hydrolase in complex with a synthetic inhibitor
Authors : Chiyo, N.; Ishii, T.; Hourai, S.; Yanagi, K.
Deposited on : 2010-09-08
Resolution : 1.98 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

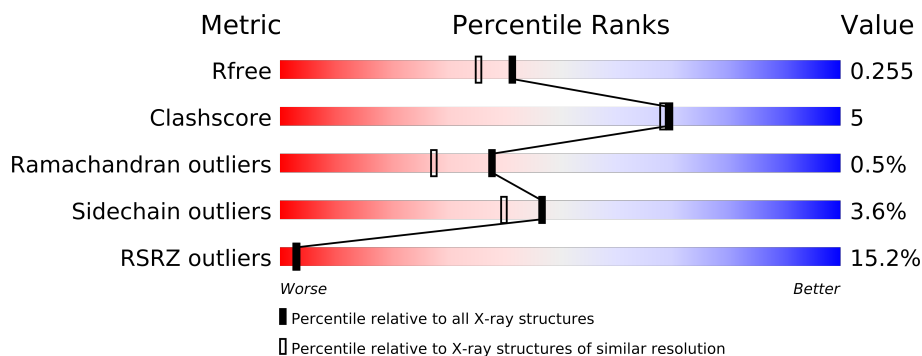
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.98 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}	66092	6577 (2.00-1.96)
Clashscore	79885	8091 (2.00-1.96)
Ramachandran outliers	78287	7989 (2.00-1.96)
Sidechain outliers	78261	7987 (2.00-1.96)
RSRZ outliers	66119	6578 (2.00-1.96)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	336	
1	B	336	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5348 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

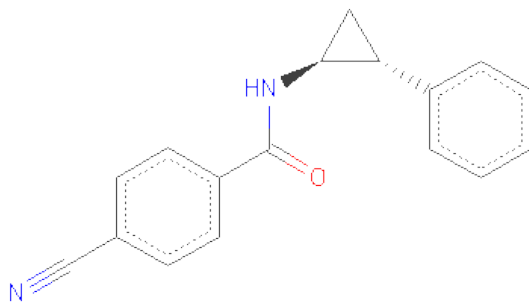
- Molecule 1 is a protein called Epoxide hydrolase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2533	1629	424	457	23			
1	B	314	Total	C	N	O	S	0	0	0
			2533	1629	424	457	23			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	MET	-	EXPRESSION TAG	UNP P34913
A	221	LYS	-	EXPRESSION TAG	UNP P34913
A	222	LYS	-	EXPRESSION TAG	UNP P34913
A	223	GLY	-	EXPRESSION TAG	UNP P34913
A	224	HIS	-	EXPRESSION TAG	UNP P34913
A	225	HIS	-	EXPRESSION TAG	UNP P34913
A	226	HIS	-	EXPRESSION TAG	UNP P34913
A	227	HIS	-	EXPRESSION TAG	UNP P34913
A	228	HIS	-	EXPRESSION TAG	UNP P34913
A	229	HIS	-	EXPRESSION TAG	UNP P34913
B	220	MET	-	EXPRESSION TAG	UNP P34913
B	221	LYS	-	EXPRESSION TAG	UNP P34913
B	222	LYS	-	EXPRESSION TAG	UNP P34913
B	223	GLY	-	EXPRESSION TAG	UNP P34913
B	224	HIS	-	EXPRESSION TAG	UNP P34913
B	225	HIS	-	EXPRESSION TAG	UNP P34913
B	226	HIS	-	EXPRESSION TAG	UNP P34913
B	227	HIS	-	EXPRESSION TAG	UNP P34913
B	228	HIS	-	EXPRESSION TAG	UNP P34913
B	229	HIS	-	EXPRESSION TAG	UNP P34913

- Molecule 2 is 4-CYANO-N-[(1S,2R)-2-PHENYLCYCLOPROPYL]BENZAMIDE (three-letter code: S38) (formula: C₁₇H₁₄N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	17	2	1		
2	B	1	Total	C	N	O	0	0
			20	17	2	1		

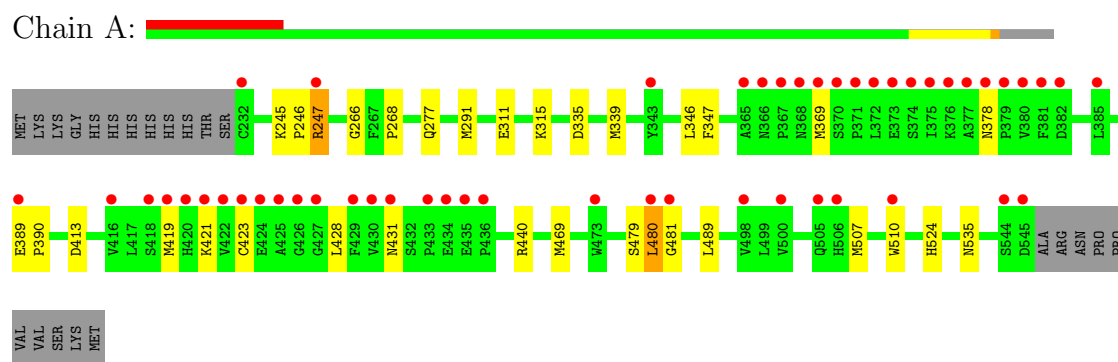
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total	O	0	0
			107	107		
3	B	135	Total	O	0	0
			135	135		

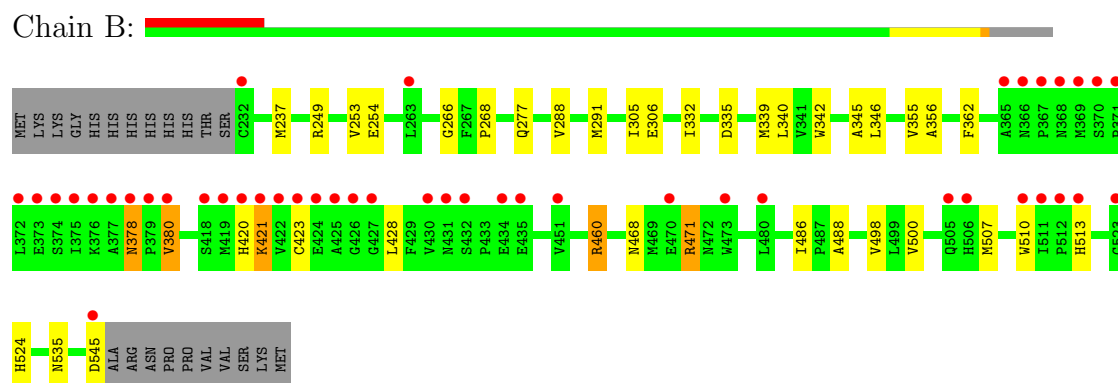
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Epoxide hydrolase 2



- Molecule 1: Epoxide hydrolase 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.63Å 80.35Å 88.69Å 90.00° 126.20° 90.00°	Depositor
Resolution (Å)	31.21 – 1.98 40.17 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.7 (31.21-1.98) 98.7 (40.17-1.98)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.76 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.219 , 0.260 0.216 , 0.255	Depositor DCC
R_{free} test set	2566 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 50573 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5348	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: S38

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	0.49	0/2609	0.59	0/3539
1	B	0.50	0/2609	0.60	1/3539 (0.0%)
All	All	0.49	0/5218	0.59	1/7078 (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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	340	LEU	CA-CB-CG	5.29	127.47	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	MET	Peptide
1	B	291	MET	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2533	0	2461	18	0
1	B	2533	0	2461	29	0
2	A	20	0	13	4	0
2	B	20	0	12	5	0
3	A	107	0	0	2	0
3	B	135	0	0	2	0
All	All	5348	0	4947	47	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (47) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:460:ARG:HH21	1:B:460:ARG:HG3	1.30	0.94
1:B:513:HIS:H	1:B:513:HIS:CD2	1.90	0.89
1:B:339:MET:CE	2:B:602:S38:N20	2.45	0.79
1:A:247:ARG:HH11	1:A:247:ARG:HG2	1.47	0.79
1:B:486:ILE:O	1:B:513:HIS:CE1	2.39	0.75
1:B:339:MET:HE2	2:B:602:S38:N20	2.05	0.71
1:B:339:MET:HE3	2:B:602:S38:N20	2.06	0.71
1:B:460:ARG:HH21	1:B:460:ARG:CG	2.05	0.68
1:B:524:HIS:NE2	2:B:602:S38:H11	2.09	0.67
1:A:524:HIS:NE2	2:A:601:S38:H11	2.15	0.62
1:B:266:GLY:HA3	1:B:335:ASP:HB3	1.81	0.62
1:A:247:ARG:CG	1:A:247:ARG:HH11	2.13	0.62
1:A:266:GLY:HA3	1:A:335:ASP:HB3	1.83	0.61
1:A:428:LEU:HD21	2:A:601:S38:H15	1.84	0.60
1:B:306:GLU:HG3	1:B:471:ARG:NH1	2.17	0.59
1:B:277:GLN:HG3	1:B:535:ASN:ND2	2.22	0.55
1:A:347:PHE:CZ	1:A:479:SER:HB3	2.41	0.55
1:A:339:MET:HE2	2:A:601:S38:N20	2.21	0.54
1:A:479:SER:O	1:A:481:GLY:N	2.41	0.53
1:A:413:ASP:OD1	1:A:440:ARG:NH2	2.39	0.53
1:A:339:MET:CE	2:A:601:S38:N20	2.72	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:500:VAL:HG12	3:B:748:HOH:O	2.10	0.49
1:B:486:ILE:O	1:B:513:HIS:HE1	1.89	0.48
1:B:355:VAL:O	1:B:488:ALA:HA	2.13	0.48
1:A:245:LYS:HB2	1:A:246:PRO:HD2	1.96	0.48
1:B:468:ASN:OD1	1:B:471:ARG:NH1	2.47	0.47
1:A:277:GLN:HG3	1:A:535:ASN:ND2	2.29	0.47
1:B:500:VAL:CG1	3:B:748:HOH:O	2.61	0.47
1:B:305:ILE:HG22	1:B:471:ARG:HH12	1.79	0.46
1:A:507:MET:HA	1:A:510:TRP:CE2	2.51	0.46
1:B:428:LEU:HD21	2:B:602:S38:H15	1.99	0.45
1:B:378:ASN:HD22	1:B:380:VAL:H	1.64	0.45
1:A:247:ARG:CG	1:A:247:ARG:NH1	2.76	0.45
1:B:460:ARG:HG3	1:B:460:ARG:NH2	2.10	0.44
1:B:420:HIS:HB2	1:B:421:LYS:HD2	2.00	0.44
1:B:306:GLU:HA	1:B:471:ARG:HH11	1.83	0.43
1:B:306:GLU:HG3	1:B:471:ARG:HH11	1.80	0.43
1:B:342:TRP:CG	1:B:362:PHE:HB2	2.54	0.42
1:B:332:ILE:HG12	1:B:356:ALA:HB3	2.02	0.42
1:B:254:GLU:HA	1:B:288:VAL:O	2.19	0.42
1:A:389:GLU:HA	1:A:390:PRO:HD3	1.92	0.42
1:A:315:LYS:HG3	3:A:755:HOH:O	2.19	0.41
1:B:345:ALA:HB1	1:B:486:ILE:HD11	2.02	0.41
1:A:311:GLU:HG2	1:A:315:LYS:HE2	2.01	0.41
1:B:237:MET:HB3	1:B:253:VAL:HG13	2.02	0.41
1:A:469:MET:SD	3:A:942:HOH:O	2.63	0.41
1:B:507:MET:HA	1:B:510:TRP:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	312/336 (93%)	300 (96%)	10 (3%)	2 (1%)	33	23
1	B	312/336 (93%)	303 (97%)	8 (3%)	1 (0%)	50	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	624/672 (93%)	603 (97%)	18 (3%)	3 (0%)	38	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	LEU
1	B	268	PRO
1	A	268	PRO

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	276/296 (93%)	266 (96%)	10 (4%)	47	40
1	B	276/296 (93%)	266 (96%)	10 (4%)	47	40
All	All	552/592 (93%)	532 (96%)	20 (4%)	47	40

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	ARG
1	A	346	LEU
1	A	369	MET
1	A	378	ASN
1	A	419	MET
1	A	421	LYS
1	A	423	CYS
1	A	431	ASN
1	A	480	LEU
1	A	489	LEU
1	B	249	ARG
1	B	346	LEU
1	B	378	ASN
1	B	380	VAL
1	B	421	LYS
1	B	423	CYS

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Mol	Chain	Res	Type
1	B	460	ARG
1	B	471	ARG
1	B	498	VAL
1	B	545	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	378	ASN
1	A	452	GLN
1	A	535	ASN
1	B	328	GLN
1	B	366	ASN
1	B	378	ASN
1	B	384	GLN
1	B	452	GLN
1	B	513	HIS
1	B	535	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	S38	A	601	-	22,22,22	0.99	1 (4%)	30,30,30	1.29	4 (13%)
2	S38	B	602	-	22,22,22	1.05	2 (9%)	30,30,30	1.24	3 (10%)

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	S38	A	601	-	-	0/14/19/19	0/2/3/3
2	S38	B	602	-	-	0/14/19/19	0/2/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	S38	C12-C10	-2.76	1.47	1.51
2	A	601	S38	C12-C10	-2.52	1.48	1.51
2	B	602	S38	C5-C7	-2.07	1.45	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	S38	C9-N8-C7	-3.04	116.34	122.92
2	A	601	S38	C9-N8-C7	-2.75	116.96	122.92
2	A	601	S38	C6-C5-C4	2.69	122.47	118.63
2	B	602	S38	C11-C9-N8	2.65	125.77	118.25
2	A	601	S38	O18-C7-C5	-2.60	116.44	121.01
2	B	602	S38	C6-C5-C4	2.52	122.23	118.63
2	A	601	S38	C3-C4-C5	-2.13	118.21	120.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	314/336 (93%)	0.99	51 (16%) 2 2	18, 31, 71, 79	0
1	B	314/336 (93%)	1.03	45 (14%) 3 3	16, 28, 70, 76	0
All	All	628/672 (93%)	1.01	96 (15%) 3 3	16, 29, 71, 79	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	372	LEU	11.6
1	A	480	LEU	9.4
1	B	372	LEU	9.2
1	B	425	ALA	8.5
1	A	375	ILE	8.4
1	B	377	ALA	8.4
1	A	377	ALA	8.3
1	B	369	MET	8.0
1	A	426	GLY	7.9
1	A	430	VAL	7.4
1	A	425	ALA	7.2
1	B	420	HIS	7.1
1	A	376	LYS	6.8
1	A	420	HIS	6.8
1	A	368	ASN	6.8
1	B	366	ASN	6.6
1	A	421	LYS	6.5
1	B	371	PRO	6.3
1	B	510	TRP	6.3
1	B	380	VAL	6.3
1	B	376	LYS	6.2
1	B	424	GLU	6.0
1	A	380	VAL	5.9
1	B	375	ILE	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	422	VAL	5.8
1	B	374	SER	5.7
1	A	369	MET	5.7
1	B	473	TRP	5.6
1	B	426	GLY	5.6
1	B	430	VAL	5.5
1	A	424	GLU	5.4
1	B	378	ASN	5.4
1	A	367	PRO	5.3
1	A	371	PRO	5.3
1	B	368	ASN	5.3
1	B	367	PRO	5.1
1	B	373	GLU	5.1
1	B	421	LYS	4.6
1	A	473	TRP	4.6
1	A	370	SER	4.3
1	B	427	GLY	4.2
1	B	370	SER	4.1
1	A	382	ASP	4.0
1	A	418	SER	4.0
1	B	434	GLU	4.0
1	B	422	VAL	4.0
1	A	379	PRO	3.9
1	A	423	CYS	3.9
1	B	512	PRO	3.8
1	A	481	GLY	3.8
1	A	427	GLY	3.8
1	A	374	SER	3.7
1	A	416	VAL	3.7
1	A	431	ASN	3.7
1	A	510	TRP	3.7
1	A	505	GLN	3.6
1	B	431	ASN	3.4
1	A	373	GLU	3.4
1	A	232	CYS	3.4
1	B	423	CYS	3.3
1	A	419	MET	3.3
1	B	506	HIS	3.3
1	A	435	GLU	3.3
1	B	379	PRO	3.2
1	B	232	CYS	3.2
1	B	432	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	545	ASP	3.1
1	B	365	ALA	3.0
1	B	513	HIS	3.0
1	A	366	ASN	3.0
1	A	506	HIS	3.0
1	A	434	GLU	3.0
1	B	263	LEU	2.9
1	A	381	PHE	2.8
1	A	378	ASN	2.8
1	B	480	LEU	2.8
1	B	435	GLU	2.7
1	A	385	LEU	2.7
1	A	365	ALA	2.6
1	A	433	PRO	2.6
1	A	429	PHE	2.6
1	B	419	MET	2.6
1	B	418	SER	2.5
1	A	436	PRO	2.5
1	B	470	GLU	2.4
1	A	247	ARG	2.3
1	A	343	TYR	2.2
1	A	544	SER	2.2
1	A	545	ASP	2.2
1	A	500	VAL	2.2
1	A	389	GLU	2.1
1	A	498	VAL	2.1
1	B	505	GLN	2.1
1	B	523	GLY	2.1
1	B	451	VAL	2.0
1	B	511	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	S38	B	602	20/20	0.21	1.40	36,40,44,44	0
2	S38	A	601	20/20	0.19	0.40	42,45,48,48	0

6.5 Other polymers

There are no such residues in this entry.